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NEWS	7	DEC 21	IPC search and display fields enhanced in CA/CAplus with the IPC reform
NEWS	8	DEC 23	New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/ USPAT2
NEWS	9	JAN 13	IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
NEWS	10	JAN 13	New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to INPADOC
NEWS	11	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS	12	JAN 17	IPC 8 in the WPI family of databases including WPIFV
NEWS	13	JAN 30	Saved answer limit increased
NEWS	14	JAN 31	Monthly current-awareness alert (SDI) frequency added to TULSA

NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
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FILE 'HOME' ENTERED AT 14:09:38 ON 14 FEB 2006

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:09:53 ON 14 FEB 2006
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 FEB 2006 HIGHEST RN 874180-50-4
DICTIONARY FILE UPDATES: 13 FEB 2006 HIGHEST RN 874180-50-4

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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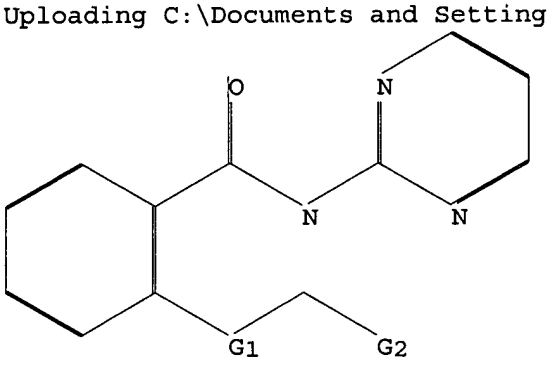
****
* *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
* *
****

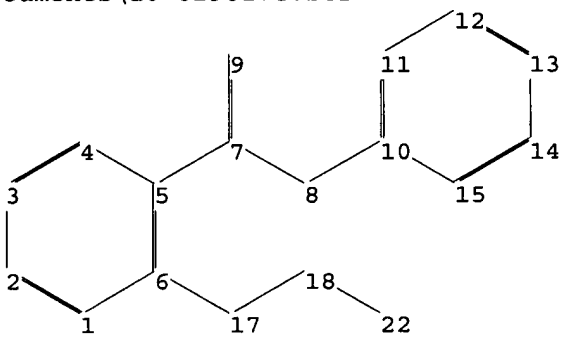
Structure search iteration limits have been increased. See HELP SLIMITS for details.

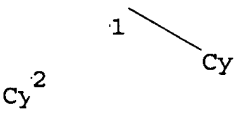
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

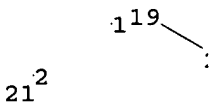
http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Documents and Settings\jballs\My Documents\10-629817G.str









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7 8 9 17 18 19 20 21 22
ring nodes :
1 2 3 4 5 6 10 11 12 13 14 15
chain bonds :
5-7 6-17 7-8 7-9 8-10 17-18 18-22 19-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15
exact/norm bonds :
6-17 7-8 7-9 8-10 17-18 18-22 19-20
exact bonds :
5-7
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

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G1:O,N

G2:O,[*1],[*2]

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:Atom  11:Atom
12:Atom  13:Atom  14:Atom  15:Atom  17:CLASS  18:CLASS  19:CLASS  20:Atom  21:Atom  22:CLASS



L1      STRUCTURE UPLOADED

=> s l1 sub sam
ENTER SUBSET L# OR (END):l1
L1 MAY NOT BE USED HERE
The L-number must have been created by a search in this file.  To see
all L-numbers defined in this session, enter DISPLAY HISTORY at an
arrow prompt (=>).  For additional information on subset searching in
this file, enter HELP SUBSET.
ENTER SUBSET L# OR (END):end
SEARCH ENDED BY USER

=> s l1
SAMPLE SEARCH INITIATED 14:10:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       18 TO ITERATE

100.0% PROCESSED       18 ITERATIONS                                  0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          106 TO      614
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.88       1.09

FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006
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FILE COVERS 1907 - 14 Feb 2006  VOL 144 ISS 8
FILE LAST UPDATED: 13 Feb 2006  (20060213/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
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=> s l1 sam
   REG1stRY INITIATED
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Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 14:11:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       18 TO ITERATE

100.0% PROCESSED       18 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          106 TO      614
PROJECTED ANSWERS:               0 TO        0

L3             0 SEA SSS SAM L1



L4           0 L3

=> s l1
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 14:12:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       18 TO ITERATE

100.0% PROCESSED       18 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          106 TO      614
PROJECTED ANSWERS:               0 TO        0

L5             0 SEA SSS SAM L1



L6           0 L5

=> s l1 full
   REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



FULL SEARCH INITIATED 14:12:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      340 TO ITERATE

100.0% PROCESSED      340 ITERATIONS                                7 ANSWERS
SEARCH TIME: 00.00.01

L7             7 SEA SSS FUL L1



L8           5 L7
```

```
=> d 1

L8   ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2006 ACS on STN
AN   2000:457059  CAPLUS
DN   133:89437
TI   Preparation of heteroaryl-substituted aromatic amides as factor Xa
     inhibitors
IN   Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman;
     Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven
     Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
     Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez,
     Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald
     Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton;
     Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PA   Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SO   PCT Int. Appl., 403 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
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PI   WO 2000039118         A1    20000706    WO 1999-US29946         19991215
         W:  AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
             IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
             MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
             SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     CA 2361149           AA    20000706    CA 1999-2361149         19991215
     EP 1140903           A1    20011010    EP 1999-964279          19991215
     EP 1140903           B1    20040804
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     JP 2002533454        T2    20021008    JP 2000-591029          19991215
     AT 272633            E     20040815    AT 1999-964279          19991215
     ES 2226485           T3    20050316    ES 1999-964279          19991215
     US 6635657           B1    20031021    US 2001-857751          20010608
     US 2004029874        A1    20040212    US 2003-629760          20030729
     US 6759414           B2    20040706
     US 2005282862        A1    20051222    US 2003-629817          20030729
PRAI US 1998-113556P      P     19981223
     WO 1999-US29946      W     19991215
     US 2001-857751       A3    20010608
OS   MARPAT 133:89437
RE.CNT  6     THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
              ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> d iall 1

L8   ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2000:457059  CAPLUS
DOCUMENT NUMBER:          133:89437
ENTRY DATE:               Entered STN:  07 Jul 2000
TITLE:                    Preparation of heteroaryl-substituted aromatic amides
                          as factor Xa inhibitors
INVENTOR(S):              Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl
                          Penman; Franciskovich, Jeffry Bernard; Goodson,
                          Theodore, Jr.; Hall, Steven Edward; Herron, David
                          Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine
                          Joseph; Masters, John Joseph; Mendel, David; Milot,
                          Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott;
                          Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe,
                          Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard
                          Crayton; Wikel, James Howard; Wiley, Michael Robert;
                          Yee, Ying Kwong
```

PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SOURCE: PCT Int. Appl., 403 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
INT. PATENT CLASSIF.:
MAIN: C07D401-14
SECONDARY: C07D401-12; C07D417-14; C07D409-14; C07D405-14; C07D213-74; A61K031-395; A61K031-435; A61K031-495; A61P007-02; C07D401-14; C07D213-00; C07D213-00; C07D211-00
CLASSIFICATION: 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 28, 63
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000039118	A1	20000706	WO 1999-US29946		19991215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2361149	AA	20000706	CA 1999-2361149		19991215
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JP 2002533454	T2	20021008	JP 2000-591029		19991215
AT 272633	E	20040815	AT 1999-964279		19991215
ES 2226485	T3	20050316	ES 1999-964279		19991215
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US 2004029874	A1	20040212	US 2003-629760		20030729
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PRIORITY APPLN. INFO.:			US 1998-113556P	P	19981223
			WO 1999-US29946	W	19991215
			US 2001-857751	A3	20010608

PATENT CLASSIFICATION CODES:

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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	ICS	C07D401-12; C07D417-14; C07D409-14; C07D405-14; C07D213-74; A61K031-395; A61K031-435; A61K031-495; A61P007-02; C07D401-14; C07D213-00; C07D213-00; C07D211-00
	IPCI	C07D0401-14 [ICM,7]; C07D0401-12 [ICS,7]; C07D0417-14 [ICS,7]; C07D0409-14 [ICS,7]; C07D0405-14 [ICS,7]; C07D0213-74 [ICS,7]; A61K0031-395 [ICS,7]; A61K0031-435 [ICS,7]; A61K0031-495 [ICS,7]; A61P0007-02 [ICS,7]; C07D0401-14 [ICS,7]; C07D0213-00 [ICS,7]; C07D0211-00 [ICS,7]
	ECLA	C07D213/75B8; C07D409/14+335+213+211; C07D417/14+277B+213+211; C07D401/12+213+205; C07D401/12+213+211; C07D401/12+213+207; C07D401/12+237B+211; C07D401/14+213+211+211; C07D401/14+213+211+205; C07D401/14+215+213+211; C07D401/14+213+213+207; C07D401/14+213+213+211; C07D401/14+233+213+211; C07D401/14+237B+213+211; C07D401/14+239B+213+211; C07D405/14+309+213+211; C07D405/14+307B+213+211; C07D409/14+333B+213+211
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	ECLA	C07D213/75B8; C07D401/12+213+207; C07D401/12+213+211; C07D401/12+213+205; C07D401/12+237B+211; C07D401/14+213+213+211; C07D401/14+213+213+207; C07D401/14+215+213+211; C07D401/14+213+211+205; C07D401/14+213+211+211; C07D401/14+239B+213+211; C07D401/14+237B+213+211; C07D401/14+233+213+211; C07D405/14+307B+213+211; C07D405/14+309+213+211; C07D409/14+335+213+211; C07D409/14+333B+213+211; C07D417/14+277B+213+211
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	ECLA	C07D213/75B8; C07D417/14+277B+213+211; C07D401/12+213+207; C07D401/12+213+211; C07D401/12+213+205; C07D401/12+237B+211; C07D401/14+213+213+211; C07D401/14+213+213+207; C07D401/14+215+213+211; C07D401/14+213+211+205; C07D401/14+213+211+211; C07D401/14+239B+213+211; C07D401/14+237B+213+211; C07D401/14+233+213+211; C07D405/14+307B+213+211; C07D405/14+309+213+211; C07D409/14+335+213+211; C07D409/14+333B+213+211
US 2005282862	IPCI	A61K0031-4545 [ICM,7]; A61K0031-4439 [ICS,7]; C07D0041-02 [ICS,7]
	NCL	514/318.000; 514/326.000; 546/194.000; 546/207.000
	ECLA	C07D213/75B8; C07D401/12+213+205; C07D401/12+213+207;

C07D401/12+213+211; C07D401/12+237B+211;
C07D401/14+213+211+205; C07D401/14+213+211+211;
C07D401/14+213+213+207; C07D401/14+213+213+211;
C07D401/14+215+213+211; C07D401/14+233+213+211;
C07D401/14+237B+213+211; C07D401/14+239B+213+211;
C07D405/14+307B+213+211; C07D405/14+309+213+211;
C07D409/14+333B+213+211; C07D409/14+335+213+211;
C07D417/14+277B+213+211

OTHER SOURCE(S): MARPAT 133:89437

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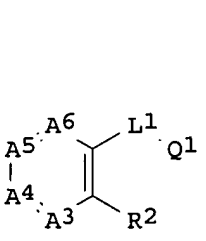

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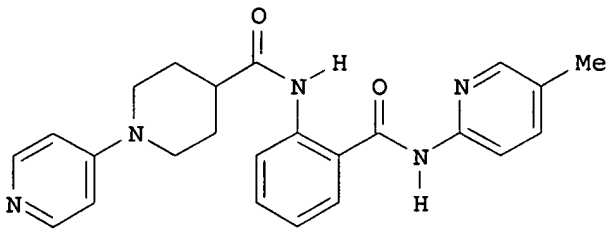

II

ABSTRACT:
The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

SUPPL. TERM: arom amide heteroaryl prepn formulation factor Xa inhibitor anticoagulant

INDEX TERM: Anticoagulants
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

INDEX TERM: 280769-11-1P 280769-16-6P 280769-22-4P 280769-23-5P
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280771-53-1P 280771-55-3P
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

INDEX TERM: 9002-05-5, Factor Xa
ROLE: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

INDEX TERM: 67-64-1, Acetone, reactions 75-64-9, tert-Butylamine, reactions 78-84-2, Isobutyraldehyde 78-93-3, Methylethyl ketone, reactions 89-98-5, 2-Chlorobenzaldehyde 96-22-0,

3-Pentanone 96-33-3 97-96-1, 2-Ethylbutyraldehyde 98-01-1, Furan-2-carboxaldehyde, reactions 98-74-8, 4-Nitrobenzenesulfonyl chloride 98-80-6, Phenylboronic acid 99-88-7, 4-Isopropylaniline 99-92-3 100-52-7, Benzaldehyde, reactions 104-88-1, 4-Chlorobenzaldehyde, reactions 105-36-2, Ethyl bromoacetate 105-58-8, Diethyl carbonate 106-47-8, 4-Chloroaniline, reactions 107-13-1, 2-Propenenitrile, reactions 108-94-1, Cyclohexanone, reactions 110-52-1, 1,4-Dibromobutane 111-42-2, reactions 120-92-3, Cyclopentanone 122-85-0, 4-Acetamidobenzaldehyde 123-11-5, 4-Methoxybenzaldehyde, reactions 123-19-3, 4-Heptanone 123-38-6, Propionaldehyde, reactions 123-75-1, Pyrrolidine, reactions 134-20-3 141-75-3, Butyryl chloride 177-11-7, 1,4-Dioxa-8-azaspiro[4.5]decane 320-98-9, 5-Fluoro-2-nitrobenzoic acid 446-10-6, 4-Fluoro-2-nitrotoluene 500-22-1, Pyridine-3-carboxaldehyde 502-42-1, Cycloheptanone 503-29-7, Azetidine 583-60-8, 2-Methylcyclohexanone 583-68-6, 2-Bromo-4-methylaniline 585-71-7, (1-Bromoethyl)benzene 587-04-2, 3-Chlorobenzaldehyde 589-16-2, 4-Ethylaniline 610-14-0, 2-Nitrobenzoyl chloride 620-23-5 701-57-5, Methyl 4-nitrophenyl sulfide 765-43-5, Cyclopropylmethylketone 769-10-8, 2-Fluoro-6-nitrotoluene 872-85-5, 4-Pyridinecarboxaldehyde 873-38-1, 2-Bromo-4-chloroaniline 1003-04-9, Tetrahydrothiophen-3-one 1003-98-1, 2-Bromo-4-fluoroaniline 1008-91-9, 1-(4-Pyridyl)piperazine 1072-72-6, Tetrahydrothiopyran-4-one 1072-98-6, 2-Amino-5-chloropyridine 1120-72-5, 2-Methylcyclopentanone 1121-60-4, Pyridine-2-carboxaldehyde 1122-54-9, 4-Acetylpyridine 1126-09-6, Ethyl isonipecotate 1489-69-6, Cyclopropanecarboxaldehyde 1603-41-4, 2-Amino-5-methylpyridine 1710-98-1, 4-tert-Butylbenzoyl chloride 1776-53-0, 4-Aminocyclohexanecarboxylic acid 1793-07-3, 2-Carbomethoxyphenyl isocyanate 1882-69-5, 5-Methoxy-2-nitrobenzoic acid 2148-56-3, 2-Amino-6-chlorobenzoic acid 2366-70-3, 4,4,4-Trifluorobutan-2-one 2516-95-2, 5-Chloro-2-nitrobenzoic acid 3113-72-2, 5-Methyl-2-nitrobenzoic acid 3678-63-5, 4-Chloro-2-picoline 4315-09-7, 4-Nitroisophthalic acid 4363-93-3, Quinoline-4-carboxaldehyde 4771-47-5, 3-Chloro-2-nitrobenzoic acid 4786-20-3, 2-Butenenitrile 4897-84-1, Methyl 4-bromobutyrate 4920-80-3, 3-Methoxy-2-nitrobenzoic acid 5350-93-6 5372-81-6, 2-Aminoterephthalic acid dimethyl ester 5428-89-7, 2-Amino-5-chloropyrimidine 5437-38-7, 3-Methyl-2-nitrobenzoic acid 5469-69-2, 3-Amino-6-chloropyridazine 5470-22-4, 4-Chloropicolinic acid 5538-51-2, Acetylsalicylic acid chloride 6280-88-2, 4-Chloro-2-nitrobenzoic acid 7304-32-7, 2-Fluoro-5-nitrobenzoic acid 7379-35-3, 4-Chloropyridine hydrochloride 7486-35-3, Tributyl(vinyl)tin 10177-29-4, 4-Chloronicotinic acid 10200-59-6, Thiazole-2-carboxaldehyde 14002-51-8, 4-Biphenylcarbonyl chloride 17012-21-4, Methyl 1-benzylpyrrolidine-3-carboxylate 19235-89-3, 4-Chloro-2-cyanopyridine 19524-06-2 21717-96-4, 2-Amino-5-fluoropyridine 29943-42-8, Tetrahydro-4H-pyran-4-one 40499-83-0, 3-Hydroxypyrrolidine 55737-66-1, 4-Methoxycarbonyl-2-nitrobenzoic acid 57260-71-6, N-tert-Butoxycarbonylpiperazine 57946-63-1, 2-Bromo-4-trifluoromethylaniline 76143-33-4, 5-Methoxycarbonyl-2-nitrobenzoic acid 79099-07-3, 1-tert-Butoxycarbonyl-4-piperidone 84358-13-4, 1-tert-Butoxycarbonyl-isonipecotic acid 93913-86-1 103057-44-9, 1-tert-Butoxycarbonyl-3-hydroxypyrrolidine 109384-19-2, 1-tert-Butoxycarbonyl-4-hydroxypiperidine 118486-94-5, 2-(Tributylstannyl)furan 124252-41-1, 4-(Tributylstannyl)pyridine 141699-55-0, 1-tert-Butoxycarbonyl-3-hydroxyazetidine 173382-28-0

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ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):

(1) Beight Douglas Wade; WO 9900121 A 1999 CAPLUS
(2) Beight Douglas Wade; WO 9900128 A 1999 CAPLUS
(3) Berlex Lab; WO 9628427 A 1996 CAPLUS
(4) Katakura; EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY CHIMICA THERAPEUTICA 1995, V30(5), P387 CAPLUS
(5) Kunitada, S; CURRENT PHARMACEUTICAL DESIGN 1996, V2(5), P6
(6) Schering Ag; WO 9932477 A 1999 CAPLUS

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L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:457059 CAPLUS
DOCUMENT NUMBER: 133:89437
TITLE: Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors
INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SOURCE: PCT Int. Appl., 403 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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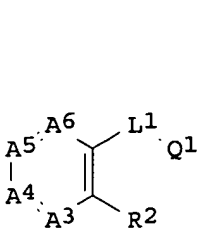
JP 2002533454	T2	20021008	JP 2000-591029	19991215
AT 272633	E	20040815	AT 1999-964279	19991215
ES 2226485	T3	20050316	ES 1999-964279	19991215
US 6635657	B1	20031021	US 2001-857751	20010608
US 2004029874	A1	20040212	US 2003-629760	20030729
US 6759414	B2	20040706		
US 2005282862	A1	20051222	US 2003-629817	20030729
PRIORITY APPLN. INFO.:			US 1998-113556P P	19981223

WO 1999-US29946 W 19991215
US 2001-857751 A3 20010608

OTHER SOURCE(S): MARPAT 133:89437

GI



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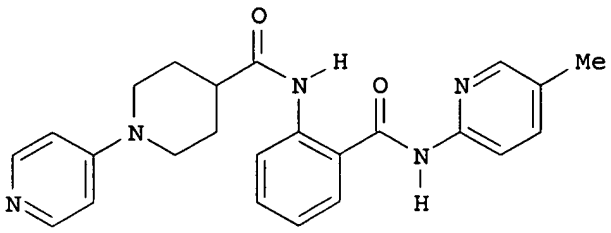


II

AB The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 14:09:38 ON 14 FEB 2006)

FILE 'REGISTRY' ENTERED AT 14:09:53 ON 14 FEB 2006
L1 STRUCTURE UPLOADED
L2 0 S L1

FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006
S L1

FILE 'REGISTRY' ENTERED AT 14:11:39 ON 14 FEB 2006
L3 0 S L1 SAM

FILE 'CAPLUS' ENTERED AT 14:11:39 ON 14 FEB 2006
L4 0 S L3 SAM
S L1

FILE 'REGISTRY' ENTERED AT 14:12:03 ON 14 FEB 2006
L5 0 S L1

FILE 'CAPLUS' ENTERED AT 14:12:03 ON 14 FEB 2006
L6 0 S L5
S L1

FILE 'REGISTRY' ENTERED AT 14:12:25 ON 14 FEB 2006
L7 7 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:12:26 ON 14 FEB 2006
L8 5 S L7 FULL

=> d l8 ibib abs

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:457059 CAPLUS
DOCUMENT NUMBER: 133:89437
TITLE: Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors

INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong

PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.

SOURCE: PCT Int. Appl., 403 pp.
CODEN: PIXXD2

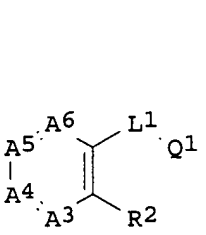
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039118	A1	20000706	WO 1999-US29946	19991215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2361149	AA	20000706	CA 1999-2361149	19991215
EP 1140903	A1	20011010	EP 1999-964279	19991215
EP 1140903	B1	20040804		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002533454	T2	20021008	JP 2000-591029	19991215
AT 272633	E	20040815	AT 1999-964279	19991215
ES 2226485	T3	20050316	ES 1999-964279	19991215
US 6635657	B1	20031021	US 2001-857751	20010608
US 2004029874	A1	20040212	US 2003-629760	20030729
US 6759414	B2	20040706		
US 2005282862	A1	20051222	US 2003-629817	20030729

PRIORITY APPLN. INFO.: US 1998-113556P P 19981223
WO 1999-US29946 W 19991215
US 2001-857751 A3 20010608

OTHER SOURCE(S): MARPAT 133:89437

GI



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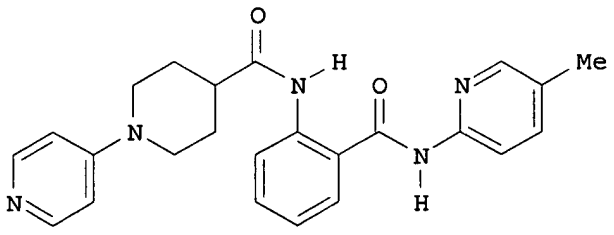


II

AB The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

```
REFERENCE COUNT:          6     THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT


=> 1
1 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d his

     (FILE 'HOME' ENTERED AT 14:09:38 ON 14 FEB 2006)

     FILE 'REGISTRY' ENTERED AT 14:09:53 ON 14 FEB 2006
L1             STRUCTURE UPLOADED
L2           0 S L1

     FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006
               S L1

     FILE 'REGISTRY' ENTERED AT 14:11:39 ON 14 FEB 2006
L3           0 S L1 SAM

     FILE 'CAPLUS' ENTERED AT 14:11:39 ON 14 FEB 2006
L4           0 S L3 SAM
               S L1

     FILE 'REGISTRY' ENTERED AT 14:12:03 ON 14 FEB 2006
L5           0 S L1

     FILE 'CAPLUS' ENTERED AT 14:12:03 ON 14 FEB 2006
L6           0 S L5
               S L1

     FILE 'REGISTRY' ENTERED AT 14:12:25 ON 14 FEB 2006
L7           7 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 14:12:26 ON 14 FEB 2006
L8           5 S L7 FULL

=> d l7 ibib abs 1-7
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y


'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
are:  (RN = CAS Registry Number)

REG    - RN
SAM    - Index Name, MF, and structure - no RN
FIDE   - All substance data, except sequence data
IDE    - FIDE, but only 50 names
SQIDE  - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD    - Protein sequence data, includes RN
SQD3   - Same as SQD, but 3-letter amino acid codes are used
SQN    - Protein sequence name information, includes RN

CALC   - Table of calculated properties
EPROP  - Table of experimental properties
PROP   - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance.  The substance formats
```

must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

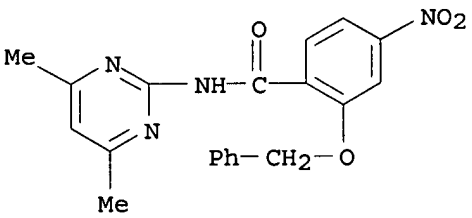
SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):ide

L7 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 856975-07-0 REGISTRY
ED Entered STN: 26 Jul 2005
CN Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H18 N4 O4
SR CAS EARLY REGISTRATIONS
LC STN Files: CA, CAPLUS

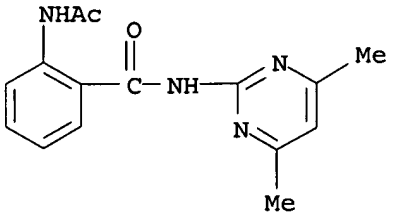


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

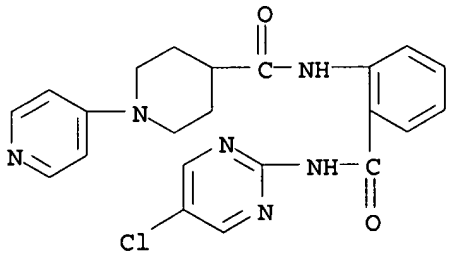
L7 ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 349622-99-7 REGISTRY
ED Entered STN: 01 Aug 2001
CN Benzamide, 2-(acetylamino)-N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H16 N4 O2
SR Chemical Library

Supplier: MicroChemistry Ltd.
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

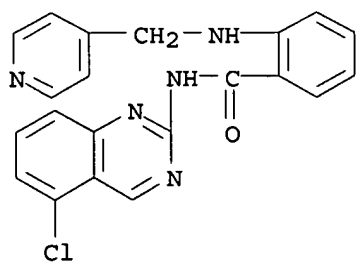
L7 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 280768-70-9 REGISTRY
ED Entered STN: 27 Jul 2000
CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phenyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H21 Cl N6 O2
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

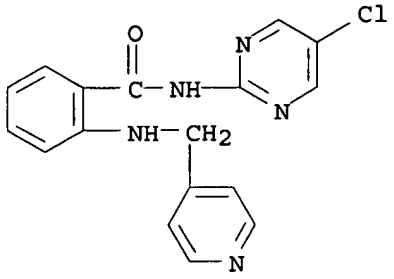
L7 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 267891-53-2 REGISTRY
ED Entered STN: 02 Jun 2000
CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H16 Cl N5 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

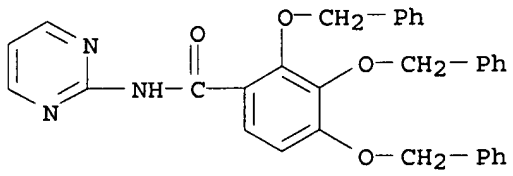
L7 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 267891-24-7 REGISTRY
ED Entered STN: 02 Jun 2000
CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H14 Cl N5 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

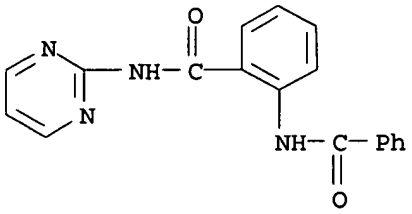
L7 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 180206-29-5 REGISTRY
ED Entered STN: 29 Aug 1996
CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H27 N3 O4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 69589-68-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H14 N4 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d his

(FILE 'HOME' ENTERED AT 14:09:38 ON 14 FEB 2006)

FILE 'REGISTRY' ENTERED AT 14:09:53 ON 14 FEB 2006
L1 STRUCTURE UPLOADED
L2 0 S L1

FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006
S L1

FILE 'REGISTRY' ENTERED AT 14:11:39 ON 14 FEB 2006
L3 0 S L1 SAM

FILE 'CAPLUS' ENTERED AT 14:11:39 ON 14 FEB 2006
L4 0 S L3 SAM
S L1

FILE 'REGISTRY' ENTERED AT 14:12:03 ON 14 FEB 2006
L5 0 S L1

FILE 'CAPLUS' ENTERED AT 14:12:03 ON 14 FEB 2006
L6 0 S L5
S L1

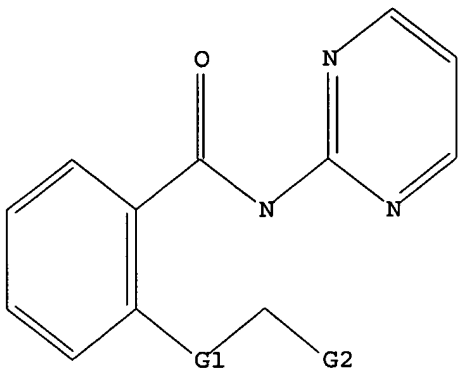
FILE 'REGISTRY' ENTERED AT 14:12:25 ON 14 FEB 2006
L7 7 S L1 FULL

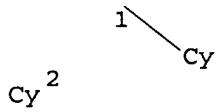
FILE 'CAPLUS' ENTERED AT 14:12:26 ON 14 FEB 2006
L8 5 S L7 FULL

FILE 'REGISTRY' ENTERED AT 14:14:45 ON 14 FEB 2006

FILE 'CAPLUS' ENTERED AT 14:14:57 ON 14 FEB 2006

=> d l1
L1 HAS NO ANSWERS
L1 STR





G1 O,N

G2 O,[@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.46	196.02

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.25

STN INTERNATIONAL LOGOFF AT 14:15:26 ON 14 FEB 2006

Connection closed by remote host

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTARJB1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	DEC 05	CASREACT(R) - Over 10 million reactions available
NEWS	4	DEC 14	2006 MeSH terms loaded in MEDLINE/LMEDLINE
NEWS	5	DEC 14	2006 MeSH terms loaded for MEDLINE file segment of TOXCENTER

```
 NEWS  6  DEC 14  CA/CAplus to be enhanced with updated IPC codes
 NEWS  7  DEC 21  IPC search and display fields enhanced in CA/CAplus with the
                  IPC reform
 NEWS  8  DEC 23  New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
                  USPAT2
 NEWS  9  JAN 13  IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
 NEWS 10  JAN 13  New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
                  INPADOC
 NEWS 11  JAN 17  Pre-1988 INPI data added to MARPAT
 NEWS 12  JAN 17  IPC 8 in the WPI family of databases including WPIFV
 NEWS 13  JAN 30  Saved answer limit increased
 NEWS 14  JAN 31  Monthly current-awareness alert (SDI) frequency
                  added to TULSA

 NEWS EXPRESS  JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
               V8.0 USERS CAN OBTAIN THE UPGRADE TO V8.01 AT
               http://download.cas.org/express/v8.0-Discover/

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS INTER    General Internet Information
 NEWS LOGIN    Welcome Banner and News Items
 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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  agreement.  Please note that this agreement limits use to scientific
  research.  Use for software development or design or implementation
  of commercial gateways or other similar uses is prohibited and may
  result in loss of user privileges and other penalties.

  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:36:32 ON 14 FEB 2006

=> file registry
COST IN U.S. DOLLARS                                SINCE FILE    TOTAL
                                                         ENTRY  SESSION
FULL ESTIMATED COST                                       0.42     0.42

FILE 'REGISTRY' ENTERED AT 14:37:27 ON 14 FEB 2006
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2006 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   13 FEB 2006  HIGHEST RN 874180-50-4
DICTIONARY FILE UPDATES:  13 FEB 2006  HIGHEST RN 874180-50-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************
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Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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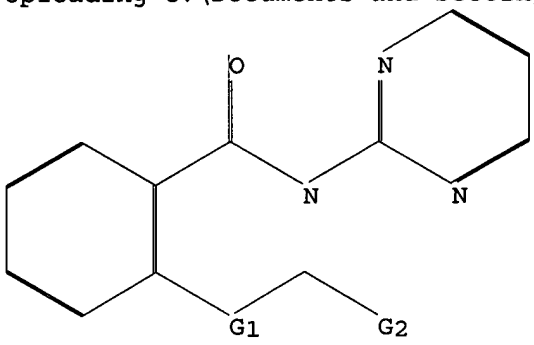
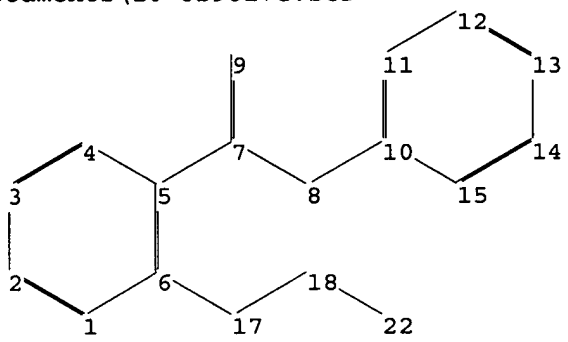
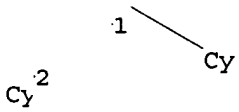
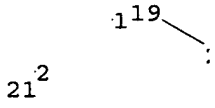
Uploading C:\Documents and Settings\jballs\My Documents\10-629817G.str









chain nodes :
7 8 9 17 18 19 20 21 22
ring nodes :
1 2 3 4 5 6 10 11 12 13 14 15
chain bonds :
5-7 6-17 7-8 7-9 8-10 17-18 18-22 19-20
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15
exact/norm bonds :
6-17 7-8 7-9 8-10 17-18 18-22 19-20
exact bonds :
5-7
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

G1:O,N

G2:O,[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 14:38:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          106 TO      614
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> file CAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                 0.44       0.86

FILE 'CAPLUS' ENTERED AT 14:38:12 ON 14 FEB 2006
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FILE COVERS 1907 - 14 Feb 2006  VOL 144 ISS 8
FILE LAST UPDATED: 13 Feb 2006  (20060213/ED)

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=> s l1
   REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




SAMPLE SEARCH INITIATED 14:38:17 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       18 TO ITERATE

100.0% PROCESSED       18 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          106 TO      614
PROJECTED ANSWERS:               0 TO        0

L3            0 SEA SSS SAM L1



L4            0 L3

=> s l1 full
   REGISTRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.
```

FULL SEARCH INITIATED 14:38:44 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 340 TO ITERATE

100.0% PROCESSED 340 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.06

L5 7 SEA SSS FUL L1

L6 5 L5

=> d l5 all abs
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L5 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 856975-07-0 REGISTRY
ED Entered STN: 26 Jul 2005
CN Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H18 N4 O4
SR CAS EARLY REGISTRATIONS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: NORL (No role in record)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
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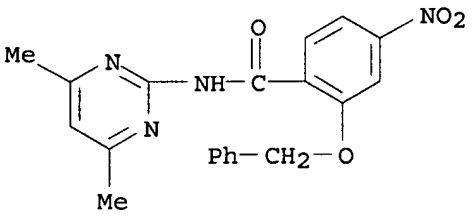
C4N2	NCNC3	6	C4N2	46.195.39	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	4.89	pH 1	(1)
Bioconc. Factor (BCF)	238	pH 4	(1)
Bioconc. Factor (BCF)	248	pH 7	(1)
Bioconc. Factor (BCF)	230	pH 8	(1)
Bioconc. Factor (BCF)	25.6	pH 10	(1)
Freely Rotatable Bonds (FRB)	7		(1)
H acceptors (HAC)	8		(1)
H donors (HD)	1		(1)

Koc (KOC)	35.4	pH 1	(1)
Koc (KOC)	1726	pH 4	(1)
Koc (KOC)	1797	pH 7	(1)
Koc (KOC)	1666	pH 8	(1)
Koc (KOC)	185	pH 10	(1)
logD (LOGD)	1.75	pH 1	(1)
logD (LOGD)	3.44	pH 4	(1)
logD (LOGD)	3.45	pH 7	(1)
logD (LOGD)	3.42	pH 8	(1)
logD (LOGD)	2.47	pH 10	(1)
logP (LOGP)	3.460+/-0.596		(1)
Molar Solubility (SLB.MOL)	0.00037 mol/L	pH 1	(1)
Molar Solubility (SLB.MOL)	0.0000076 mol/L	pH 4	(1)
Molar Solubility (SLB.MOL)	0.0000073 mol/L	pH 7	(1)
Molar Solubility (SLB.MOL)	0.0000078 mol/L	pH 8	(1)
Molar Solubility (SLB.MOL)	0.000070 mol/L	pH 10	(1)
Molecular Weight (MW)	378.38		(1)
pKa (PKA)	9.05+/-0.70	Most Acidic	(1)
pKa (PKA)	2.70+/-0.17	Most Basic	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V4.76 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 47:22216 CA
TI Tuberculostatic derivatives of p-aminobenzoic acid. III. Heterocyclic derivatives of 4-aminosalicylic acid
AU Jensen, Kai Arne; Ingvorsen, Helmuth
CS Univ. Copenhagen
SO Acta Chemica Scandinavica (1952), 6, 161-5
CODEN: ACHSE7; ISSN: 0904-213X
DT Journal
LA English
CC 10 (Organic Chemistry)
AB cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and 4-aminosalicylic acid (II) were prepared, including 4-nitro-salicylomorpholide (III), m. 247-8°, and -piperidide (IV), m. 230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m. 170° and 4-aminobenzoic acid (VIII), m. 160°; 2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X), m. 178°, and -benzanilide (XI), m. 201°; 4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-nitrobenzamido)pyridine (XIII), m. 144°, -thiazole (XIV), m. 201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4-aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m. 214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et 4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at 120°, the excess XX removed at 100° in vacuo, the residue dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving 50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g. PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were refluxed until colorless, 0.2 N NaOH added until the color reappeared, the EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5 h., the excess SOCl2 was removed in vacuo, and the IX (9.2 g.) treated with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the

solution filtered, part of the EtOH removed in vacuo, H2O added, the solution heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9 g. acid chloride. XVII to XIX were obtained by hydrogenation of the corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.

IT Heterocyclic compounds
Heterocyclic compounds
Heterocyclic compounds
Heterocyclic compounds

IT Salicylamide, 4-nitro-N-2-pyridyl-
Salicylamide, N-(5-methyl-1,3,4-thiadiazol-2-yl)-4-nitro-
Salicylanilide, 4-nitro-4'-sulfamoyl-

IT 65-49-6, Salicylic acid, 4-amino- 150-13-0, Benzoic acid, p-amino- (derivs.)

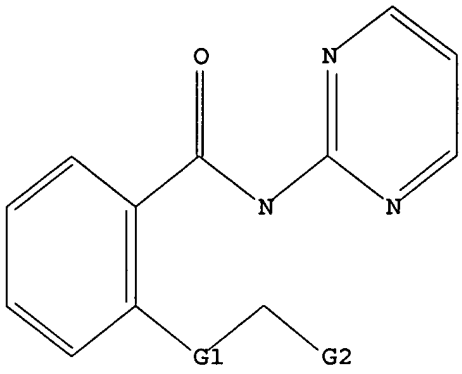
IT 5340-21-6, Benzoic acid, 2-(benzyloxy)-4-nitro- 6935-15-5, Salicylic acid, 4-carboxyamino-, 4-benzyl ester 39614-82-9, Salicyloyl chloride, 4-nitro- 78154-65-1, Salicylanilide, 4-amino- 78154-68-4, Morpholine, 4-(4-nitrosalicyloyl)- 78154-68-4, Phenol, 2-morpholinocarbonyl-5-nitro- 78154-69-5, Piperidine, 1-(4-nitrosalicyloyl)- 78154-69-5, Phenol, 5-nitro-2-piperidinocarbonyl- 78154-70-8, Morpholine, 4-(4-aminosalicyloyl)- 78154-71-9, Phenol, 5-amino-2-piperidinocarbonyl- 78154-71-9, Piperidine, 1-(4-aminosalicyloyl)- 99072-94-3, Salicylamide, 4-amino-N-(5-methyl-1,3,4-thiadiazol-2-yl)- 99185-78-1, Salicylamide, 4-amino-N-2-thiazolyl- 99989-22-7, Salicylamide, 4-amino-N-2-pyridyl- 100872-84-2, Benzamide, 2-(benzyloxy)-4-nitro- 106952-12-9, Salicylanilide, 4',4'''-sulfonylbis[4-amino- 109016-83-3, Salicylanilide, 4-amino-4'-sulfamoyl- 193803-83-7, Benzoic acid, 4-amino-2-(benzyloxy)- 607713-82-6, Benzoyl chloride, 2-(benzyloxy)-4-nitro- 721920-30-5, 5-Thiazolecarboxylic acid, 4-methyl-2-(4-nitrosalicylamido)-, ethyl ester 850852-03-8, Thiazole, 2-[2-(benzyloxy)-4-nitrobenzamido]- 856848-98-1, Pyridine, 2-[2-(benzyloxy)-4-nitrobenzamido]- 856861-93-3, Salicylamide, 4-nitro-N-s-triazol-3-yl- 856975-07-0, Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- 857533-50-7, Benzanilide, 4-amino-2-(benzyloxy)- 857534-05-5, Benzanilide, 2-(benzyloxy)-4-nitro- 857748-51-7, 1,3,4-Thiadiazole, 2-[4-amino-2-(benzyloxy)benzamido]-5-methyl- 857748-52-8, 1,3,4-Thiadiazole, 2-[2-(benzyloxy)-4-nitrobenzamido]-5-methyl- 857749-06-5, 1,3,4-Thiadiazole, 2-methyl-5-[N4-(4-nitrosalicyloyl)sulfanilamido]- 857749-06-5, Salicylanilide, 4'-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfamoyl]-4-nitro- 857756-40-2, Salicylamide, N-(4,5-dimethyl-2-thiazolyl)-4-nitro- 857756-48-0, Salicylamide, 4-nitro-N-p-sulfamoylbenzyl- 857756-83-3, Salicylanilide, 4-amino-4'-(2-thiazolylsulfamoyl)- 857757-02-9, Salicylanilide, 4'-[(4-methyl-2-pyrimidinyl)sulfamoyl]-4-nitro- 857757-02-9, Pyrimidine, 4-methyl-2-[N4-(4-nitrosalicyloyl)sulfanilamido]- 857757-06-3, Salicylanilide, 4-nitro-4'-(2-thiazolylsulfamoyl)- 857757-06-3, Thiazole, 2-[N4-(4-nitrosalicyloyl)sulfanilamido]- 858479-10-4, Salicylamide, 4-nitro-N-2-thiazolyl- 858479-45-5, Salicylamide, 4-amino-N-p-sulfamoylbenzyl- 858479-46-6, Salicylanilide, 4-nitro-4'-(2-pyrimidinylsulfamoyl)- 858479-47-7, Salicylanilide, 4-nitro-4'-(2-pyridylsulfamoyl)- 858479-65-9, Salicylanilide, 4-amino-4'-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfamoyl]- 858479-65-9, 1,3,4-Thiadiazole, 2-[N4-(4-aminosalicyloyl)sulfanilamido]-5-methyl- 859466-83-4, Thiazole, 2-[4-amino-2-(benzyloxy)benzamido]- 860507-31-9, Salicylamide, 4-amino-N-(4,5-dimethyl-2-thiazolyl)- 860507-36-4, Salicylanilide, 4',4'''-sulfonylbis[4-nitro- 867131-41-7, Pyridine, 2-[4-amino-2-(benzyloxy)benzamido]- 873401-46-8, 1,3,4-Thiadiazole, 2-methyl-5-(4-nitrosalicylamido)-
(preparation of)

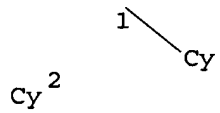
AB cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and 4-aminosalicylic acid (II) were prepared, including 4-nitrosalicylomorpholide (III), m. 247-8°, and -piperidide (IV), m. 230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m. 170° and 4-aminobenzoic acid (VIII), m. 160°; 2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X), m. 178°, and -benzanilide (XI), m. 201°; 4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-nitrobenzamido)pyridine (XIII), m. 144°, -thiazole (XIV), m.

201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4-aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m. 214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et 4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at 120°, the excess XX removed at 100° in vacuo, the residue dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving 50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g. PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were refluxed until colorless, 0.2 N NaOH added until the color reappeared, the EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5 h., the excess SOCl2 was removed in vacuo, and the IX (9.2 g.) treated with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the solution filtered, part of the EtOH removed in vacuo, H2O added, the solution heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9 g. acid chloride. XVII to XIX were obtained by hydrogenation of the corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.

```
=> s l1 full 2
   REGIstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




SAMPLE SEARCH INITIATED 14:39:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       18 TO ITERATE

100.0% PROCESSED       18 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          106 TO      614
PROJECTED ANSWERS:               0 TO        0

L7             0 SEA SSS SAM L1



L8             0 L7


MISSING OPERATOR L8 FULL
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> d l1 full 2
L1 HAS NO ANSWERS
'FULL ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
          data.  (Default)
SIM ----- Structure IMage.
SAT ----- Structure ATtributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
          data.
SDA ----- All Structure DAta (image, attributes, connection table and
```

map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:sim
L1 STR





G1 O,N

G2 O,[@1],[@2]

Structure attributes must be viewed using STN Express query preparation.

=> d l5 ibib abs 1-7
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats. The predefined substance formats
are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance. The substance formats
must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data

CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB ------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

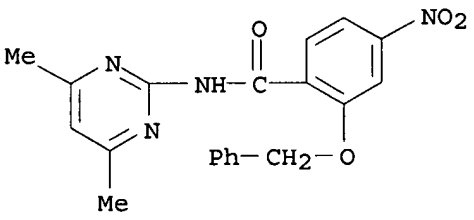
SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):ide

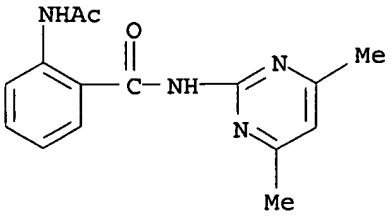
L5   ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN   856975-07-0 REGISTRY
ED   Entered STN: 26 Jul 2005
CN   Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA
     INDEX NAME)
FS   3D CONCORD
MF   C20 H18 N4 O4
SR   CAS EARLY REGISTRATIONS
LC   STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

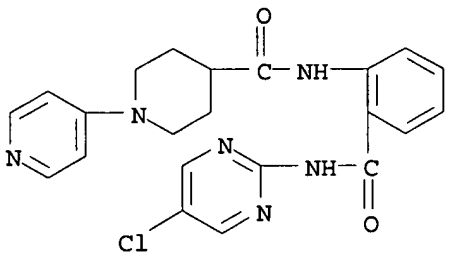
               1 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5   ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN   349622-99-7 REGISTRY
ED   Entered STN: 01 Aug 2001
CN   Benzamide, 2-(acetylamino)-N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA
     INDEX NAME)
FS   3D CONCORD
MF   C15 H16 N4 O2
SR   Chemical Library
       Supplier: MicroChemistry Ltd.
LC   STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

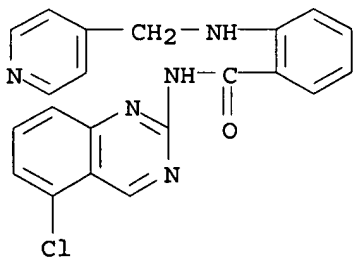
L5 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 280768-70-9 REGISTRY
ED Entered STN: 27 Jul 2000
CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phenyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H21 Cl N6 O2
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

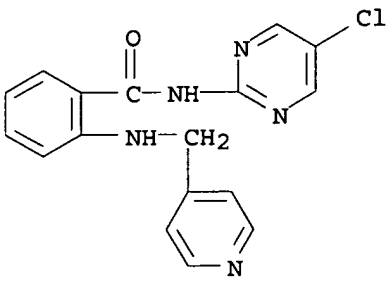
L5 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 267891-53-2 REGISTRY
ED Entered STN: 02 Jun 2000
CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H16 Cl N5 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

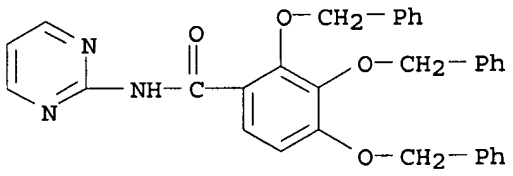
L5 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 267891-24-7 REGISTRY
ED Entered STN: 02 Jun 2000
CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H14 Cl N5 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

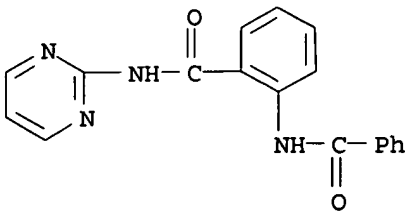
L5 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 180206-29-5 REGISTRY
ED Entered STN: 29 Aug 1996
CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H27 N3 O4
SR CA
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 69589-68-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H14 N4 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

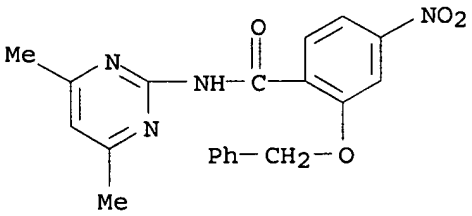
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d l5 all 1-7
YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

L5 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 856975-07-0 REGISTRY
ED Entered STN: 26 Jul 2005
CN Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H18 N4 O4
SR CAS EARLY REGISTRATIONS
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: NORL (No role in record)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2
C4N2	NCNC3	6	C4N2	46.195.39	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	4.89	pH 1	(1)
Bioconc. Factor (BCF)	238	pH 4	(1)
Bioconc. Factor (BCF)	248	pH 7	(1)
Bioconc. Factor (BCF)	230	pH 8	(1)

Bioconc. Factor (BCF)	25.6	pH 10	(1)
Freely Rotatable Bonds (FRB)	7		(1)
H acceptors (HAC)	8		(1)
H donors (HD)	1		(1)
Koc (KOC)	35.4	pH 1	(1)
Koc (KOC)	1726	pH 4	(1)
Koc (KOC)	1797	pH 7	(1)
Koc (KOC)	1666	pH 8	(1)
Koc (KOC)	185	pH 10	(1)
logD (LOGD)	1.75	pH 1	(1)
logD (LOGD)	3.44	pH 4	(1)
logD (LOGD)	3.45	pH 7	(1)
logD (LOGD)	3.42	pH 8	(1)
logD (LOGD)	2.47	pH 10	(1)
logP (LOGP)	3.460+/-0.596		(1)
Molar Solubility (SLB.MOL)	0.00037 mol/L	pH 1	(1)
Molar Solubility (SLB.MOL)	0.0000076 mol/L	pH 4	(1)
Molar Solubility (SLB.MOL)	0.0000073 mol/L	pH 7	(1)
Molar Solubility (SLB.MOL)	0.0000078 mol/L	pH 8	(1)
Molar Solubility (SLB.MOL)	0.000070 mol/L	pH 10	(1)
Molecular Weight (MW)	378.38		(1)
pKa (PKA)	9.05+/-0.70	Most Acidic	(1)
pKa (PKA)	2.70+/-0.17	Most Basic	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V4.76 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 47:22216 CA
TI Tuberculostatic derivatives of p-aminobenzoic acid. III. Heterocyclic derivatives of 4-aminosalicylic acid
AU Jensen, Kai Arne; Ingvorsen, Helmuth
CS Univ. Copenhagen
SO Acta Chemica Scandinavica (1952), 6, 161-5
CODEN: ACHSE7; ISSN: 0904-213X
DT Journal
LA English
CC 10 (Organic Chemistry)
AB cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and 4-aminosalicylic acid (II) were prepared, including 4-nitro-salicylomorpholide (III), m. 247-8°, and -piperidide (IV), m. 230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m. 170° and 4-aminobenzoic acid (VIII), m. 160°; 2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X), m. 178°, and -benzanilide (XI), m. 201°; 4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-nitrobenzamido)pyridine (XIII), m. 144°, -thiazole (XIV), m. 201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4-aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m. 214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et 4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at 120°, the excess XX removed at 100° in vacuo, the residue dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving 50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g. PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were refluxed until colorless, 0.2 N NaOH added until the color reappeared, the EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5 h., the excess SOCl2 was removed in vacuo, and the IX (9.2 g.) treated

with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the solution filtered, part of the EtOH removed in vacuo, H2O added, the solution heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9 g. acid chloride. XVII to XIX were obtained by hydrogenation of the corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.

IT Heterocyclic compounds
Heterocyclic compounds
Heterocyclic compounds
Heterocyclic compounds

IT Salicylamide, 4-nitro-N-2-pyridyl-
Salicylamide, N-(5-methyl-1,3,4-thiadiazol-2-yl)-4-nitro-
Salicylanilide, 4-nitro-4'-sulfamoyl-

IT 65-49-6, Salicylic acid, 4-amino- 150-13-0, Benzoic acid, p-amino- (derivs.)

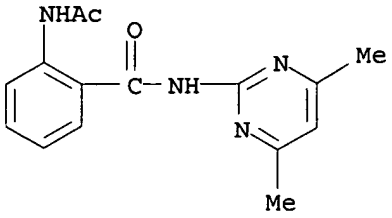
IT 5340-21-6, Benzoic acid, 2-(benzyloxy)-4-nitro- 6935-15-5, Salicylic acid, 4-carboxyamino-, 4-benzyl ester 39614-82-9, Salicyloyl chloride, 4-nitro- 78154-65-1, Salicylanilide, 4-amino- 78154-68-4, Morpholine, 4-(4-nitrosalicyloyl)- 78154-68-4, Phenol, 2-morpholinocarbonyl-5-nitro- 78154-69-5, Piperidine, 1-(4-nitrosalicyloyl)- 78154-69-5, Phenol, 5-nitro-2-piperidinocarbonyl- 78154-70-8, Morpholine, 4-(4-aminosalicyloyl)- 78154-71-9, Phenol, 5-amino-2-piperidinocarbonyl- 78154-71-9, Piperidine, 1-(4-aminosalicyloyl)- 99072-94-3, Salicylamide, 4-amino-N-(5-methyl-1,3,4-thiadiazol-2-yl)- 99185-78-1, Salicylamide, 4-amino-N-2-thiazolyl- 99989-22-7, Salicylamide, 4-amino-N-2-pyridyl- 100872-84-2, Benzamide, 2-(benzyloxy)-4-nitro- 106952-12-9, Salicylanilide, 4',4'''-sulfonylbis[4-amino- 109016-83-3, Salicylanilide, 4-amino-4'-sulfamoyl- 193803-83-7, Benzoic acid, 4-amino-2-(benzyloxy)- 607713-82-6, Benzoyl chloride, 2-(benzyloxy)-4-nitro- 721920-30-5, 5-Thiazolecarboxylic acid, 4-methyl-2-(4-nitrosalicylamido)-, ethyl ester 850852-03-8, Thiazole, 2-[2-(benzyloxy)-4-nitrobenzamido]- 856848-98-1, Pyridine, 2-[2-(benzyloxy)-4-nitrobenzamido]- 856861-93-3, Salicylamide, 4-nitro-N-s-triazol-3-yl- 856975-07-0, Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- 857533-50-7, Benzanilide, 4-amino-2-(benzyloxy)- 857534-05-5, Benzanilide, 2-(benzyloxy)-4-nitro- 857748-51-7, 1,3,4-Thiadiazole, 2-[4-amino-2-(benzyloxy)benzamido]-5-methyl- 857748-52-8, 1,3,4-Thiadiazole, 2-[2-(benzyloxy)-4-nitrobenzamido]-5-methyl- 857749-06-5, 1,3,4-Thiadiazole, 2-methyl-5-[N4-(4-nitrosalicyloyl)sulfanilamido]- 857749-06-5, Salicylanilide, 4'-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfamoyl]-4-nitro- 857756-40-2, Salicylamide, N-(4,5-dimethyl-2-thiazolyl)-4-nitro- 857756-48-0, Salicylamide, 4-nitro-N-p-sulfamoylbenzyl- 857756-83-3, Salicylanilide, 4-amino-4'-(2-thiazolylsulfamoyl)- 857757-02-9, Salicylanilide, 4'-[(4-methyl-2-pyrimidinyl)sulfamoyl]-4-nitro- 857757-02-9, Pyrimidine, 4-methyl-2-[N4-(4-nitrosalicyloyl)sulfanilamido]- 857757-06-3, Salicylanilide, 4-nitro-4'-(2-thiazolylsulfamoyl)- 857757-06-3, Thiazole, 2-[N4-(4-nitrosalicyloyl)sulfanilamido]- 858479-10-4, Salicylamide, 4-nitro-N-2-thiazolyl- 858479-45-5, Salicylamide, 4-amino-N-p-sulfamoylbenzyl- 858479-46-6, Salicylanilide, 4-nitro-4'-(2-pyrimidinylsulfamoyl)- 858479-47-7, Salicylanilide, 4-nitro-4'-(2-pyridylsulfamoyl)- 858479-65-9, Salicylanilide, 4-amino-4'-[(5-methyl-1,3,4-thiadiazol-2-yl)sulfamoyl]- 858479-65-9, 1,3,4-Thiadiazole, 2-[N4-(4-aminosalicyloyl)sulfanilamido]-5-methyl- 859466-83-4, Thiazole, 2-[4-amino-2-(benzyloxy)benzamido]- 860507-31-9, Salicylamide, 4-amino-N-(4,5-dimethyl-2-thiazolyl)- 860507-36-4, Salicylanilide, 4',4'''-sulfonylbis[4-nitro- 867131-41-7, Pyridine, 2-[4-amino-2-(benzyloxy)benzamido]- 873401-46-8, 1,3,4-Thiadiazole, 2-methyl-5-(4-nitrosalicylamido)-
(preparation of)

L5 ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 349622-99-7 REGISTRY
ED Entered STN: 01 Aug 2001
CN Benzamide, 2-(acetylamino)-N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)

FS 3D CONCORD
MF C15 H16 N4 O2
SR Chemical Library
      Supplier: MicroChemistry Ltd.
LC STN Files: CHEMCATS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C4N2	NCNC3	6	C4N2	46.195.39	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.07	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	6.15	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	12.10	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	13.40	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	13.55	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	13.56	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	13.56	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	13.52	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	13.11	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	10.08	pH 10 25 deg C	(1)
Density (DEN)	1.290+/-0.06 g/cm**3	760 Torr	(1)
Freely Rotatable Bonds (FRB)	2		(1)
H acceptors (HAC)	6		(1)
H donors (HD)	2		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	8		(1)
Koc (KOC)	17.75	pH 1 25 deg C	(1)
Koc (KOC)	101.91	pH 2 25 deg C	(1)
Koc (KOC)	200.58	pH 3 25 deg C	(1)
Koc (KOC)	222.17	pH 4 25 deg C	(1)
Koc (KOC)	224.59	pH 5 25 deg C	(1)
Koc (KOC)	224.82	pH 6 25 deg C	(1)
Koc (KOC)	224.78	pH 7 25 deg C	(1)
Koc (KOC)	224.08	pH 8 25 deg C	(1)
Koc (KOC)	217.33	pH 9 25 deg C	(1)
Koc (KOC)	167.13	pH 10 25 deg C	(1)
logD (LOGD)	0.69	pH 1 25 deg C	(1)
logD (LOGD)	1.45	pH 2 25 deg C	(1)
logD (LOGD)	1.74	pH 3 25 deg C	(1)
logD (LOGD)	1.79	pH 4 25 deg C	(1)
logD (LOGD)	1.79	pH 5 25 deg C	(1)
logD (LOGD)	1.79	pH 6 25 deg C	(1)
logD (LOGD)	1.79	pH 7 25 deg C	(1)

logD (LOGD)	1.79	pH 8 25 deg C	(1)
logD (LOGD)	1.78	pH 9 25 deg C	(1)
logD (LOGD)	1.66	pH 10 25 deg C	(1)
logP (LOGP)	1.793+/-0.598	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.12 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	1.5 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.27 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.14 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.12 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.12 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.12 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.12 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.12 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.13 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.16 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.12 g/L	Unbuffered Water pH 6.81 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.00042 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0054 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00094 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00048 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00043 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00042 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00042 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00042 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00043 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00044 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00057 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00042 mol/L	Unbuffered Water pH 6.81 25 deg C	(1)
Molar Volume (MVOL)	220.3+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	284.31		(1)
pKa (PKA)	10.46+/-0.70	Most Acidic 25 deg C	(1)
pKa (PKA)	2.08+/-0.50	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	83.98 A**2		(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19 ((C) 1994-2006 ACD/Labs)

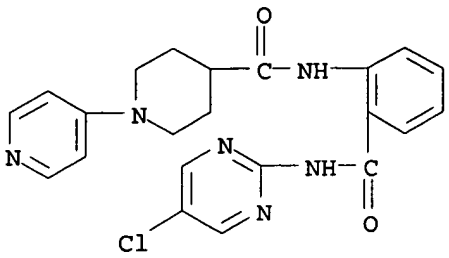
See HELP PROPERTIES for information about property data sources in REGISTRY.

L5 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 280768-70-9 REGISTRY
ED Entered STN: 27 Jul 2000
CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phenyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H21 Cl N6 O2
SR CA
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N	NC5	6	C5N	46.156.1	1

C5N	NC5	6	C5N	46.156.30	1
C4N2	NCNC3	6	C4N2	46.195.39	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	1.70	pH 10 25 deg C	(1)
Density (DEN)	1.405+/-0.06 g/cm**3	760 Torr	(1)
Freely Rotatable Bonds (FRB)	4		(1)
H acceptors (HAC)	8		(1)
H donors (HD)	2		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	10		(1)
Koc (KOC)	1.73	pH 1 25 deg C	(1)
Koc (KOC)	1.75	pH 2 25 deg C	(1)
Koc (KOC)	1.76	pH 3 25 deg C	(1)
Koc (KOC)	1.76	pH 4 25 deg C	(1)
Koc (KOC)	1.76	pH 5 25 deg C	(1)
Koc (KOC)	1.76	pH 6 25 deg C	(1)
Koc (KOC)	1.83	pH 7 25 deg C	(1)
Koc (KOC)	2.47	pH 8 25 deg C	(1)
Koc (KOC)	7.46	pH 9 25 deg C	(1)
Koc (KOC)	19.72	pH 10 25 deg C	(1)
logD (LOGD)	0.01	pH 1 25 deg C	(1)
logD (LOGD)	0.01	pH 2 25 deg C	(1)
logD (LOGD)	0.01	pH 3 25 deg C	(1)
logD (LOGD)	0.01	pH 4 25 deg C	(1)
logD (LOGD)	0.01	pH 5 25 deg C	(1)
logD (LOGD)	0.02	pH 6 25 deg C	(1)
logD (LOGD)	0.03	pH 7 25 deg C	(1)
logD (LOGD)	0.16	pH 8 25 deg C	(1)
logD (LOGD)	0.64	pH 9 25 deg C	(1)
logD (LOGD)	1.06	pH 10 25 deg C	(1)
logP (LOGP)	2.514+/-0.646	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.011 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	3.7 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	3.6 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	3.6 g/L	pH 3 25 deg C	(1)

Mass Solubility (SLB.MASS)	3.6 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	3.6 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	3.4 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	2.3 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.57 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.079 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.026 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.035 g/L	Unbuffered Water	(1)
		pH 9.57	
		25 deg C	
Molar Intrinsic Solubility (ISLB.MOL)	0.000026 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0084 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0083 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0083 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0083 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0082 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0078 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0053 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0013 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00018 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000059 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000080 mol/L	Unbuffered Water	(1)
		pH 9.57	
		25 deg C	
Molar Volume (MVOL)	310.7+/-3.0 cm**3/mol	20 deg C	(1)
		760 Torr	
Molecular Weight (MW)	436.89		(1)
pKa (PKA)	9.58+/-0.70	Most Acidic	(1)
		25 deg C	
pKa (PKA)	10.88+/-0.10	Most Basic	(1)
		25 deg C	
Polar Surface Area (PSA)	100.11 A**2		(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 133:89437 CA
TI Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors
IN Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PA Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SO PCT Int. Appl., 403 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D401-14
ICS C07D401-12; C07D417-14; C07D409-14; C07D405-14; C07D213-74; A61K031-395; A61K031-435; A61K031-495; A61P007-02; C07D401-14; C07D213-00; C07D213-00; C07D211-00
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 28, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2000039118	A1	20000706	WO 1999-US29946	19991215

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CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
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CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2361149	AA	20000706	CA 1999-2361149	19991215
EP 1140903	A1	20011010	EP 1999-964279	19991215
EP 1140903	B1	20040804		
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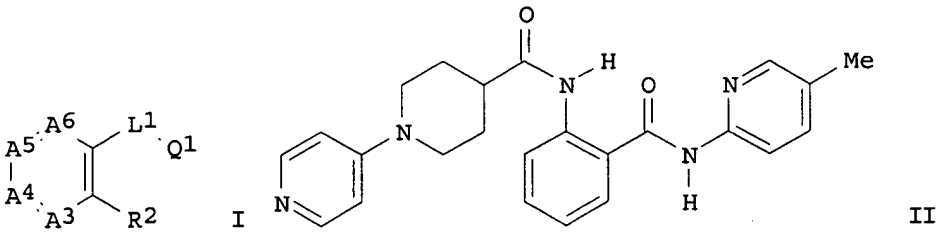
AT 272633	E	20040815	AT 1999-964279	19991215
ES 2226485	T3	20050316	ES 1999-964279	19991215
US 6635657	B1	20031021	US 2001-857751	20010608
US 2004029874	A1	20040212	US 2003-629760	20030729
US 6759414	B2	20040706		
US 2005282862	A1	20051222	US 2003-629817	20030729

PRAI US 1998-113556P 19981223
WO 1999-US29946 19991215
US 2001-857751 20010608

GI



AB The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

ST arom amide heteroaryl prepn formulation factor Xa inhibitor anticoagulant

IT Anticoagulants
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

IT 280769-11-1P 280769-16-6P 280769-22-4P 280769-23-5P 280769-24-6P
280769-46-2P 280769-59-7P 280769-68-8P 280769-83-7P 280770-51-6P
280770-52-7P 280770-59-4P 280770-66-3P 280770-79-8P 280770-91-4P
280770-93-6P 280770-95-8P 280771-19-9P 280771-47-3P 280771-49-5P
280771-53-1P 280771-55-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

IT 280768-65-2P 280768-66-3P 280768-67-4P 280768-68-5P 280768-69-6P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

IT 280771-27-9P 280771-28-0P 280771-29-1P 280771-30-4P 280771-31-5P
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280771-37-1P 280771-38-2P 280771-39-3P 280771-40-6P 280771-41-7P
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280771-48-4P 280771-50-8P 280771-51-9P 280771-52-0P 280771-54-2P
280771-56-4P 280771-57-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

IT 9002-05-5, Factor Xa
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

IT 67-64-1, Acetone, reactions 75-64-9, tert-Butylamine, reactions
78-84-2, Isobutyraldehyde 78-93-3, Methylethyl ketone, reactions
89-98-5, 2-Chlorobenzaldehyde 96-22-0, 3-Pentanone 96-33-3 97-96-1,
2-Ethylbutyraldehyde 98-01-1, Furan-2-carboxaldehyde, reactions
98-74-8, 4-Nitrobenzenesulfonyl chloride 98-80-6, Phenylboronic acid
99-88-7, 4-Isopropylaniline 99-92-3 100-52-7, Benzaldehyde, reactions
104-88-1, 4-Chlorobenzaldehyde, reactions 105-36-2, Ethyl bromoacetate
105-58-8, Diethyl carbonate 106-47-8, 4-Chloroaniline, reactions
107-13-1, 2-Propenenitrile, reactions 108-94-1, Cyclohexanone, reactions
110-52-1, 1,4-Dibromobutane 111-42-2, reactions 120-92-3,
Cyclopentanone 122-85-0, 4-Acetamidobenzaldehyde 123-11-5,
4-Methoxybenzaldehyde, reactions 123-19-3, 4-Heptanone 123-38-6,
Propionaldehyde, reactions 123-75-1, Pyrrolidine, reactions 134-20-3

141-75-3, Butyryl chloride 177-11-7, 1,4-Dioxa-8-azaspiro[4.5]decane
320-98-9, 5-Fluoro-2-nitrobenzoic acid 446-10-6, 4-Fluoro-2-nitrotoluene
500-22-1, Pyridine-3-carboxaldehyde 502-42-1, Cycloheptanone
503-29-7, Azetidine 583-60-8, 2-Methylcyclohexanone 583-68-6,
2-Bromo-4-methylaniline 585-71-7, (1-Bromoethyl)benzene 587-04-2,
3-Chlorobenzaldehyde 589-16-2, 4-Ethylaniline 610-14-0, 2-Nitrobenzoyl
chloride 620-23-5 701-57-5, Methyl 4-nitrophenyl sulfide 765-43-5,
Cyclopropylmethylketone 769-10-8, 2-Fluoro-6-nitrotoluene 872-85-5,
4-Pyridinecarboxaldehyde 873-38-1, 2-Bromo-4-chloroaniline 1003-04-9,
Tetrahydrothiophen-3-one 1003-98-1, 2-Bromo-4-fluoroaniline 1008-91-9,
1-(4-Pyridyl)piperazine 1072-72-6, Tetrahydrothiopyran-4-one 1072-98-6
, 2-Amino-5-chloropyridine 1120-72-5, 2-Methylcyclopentanone 1121-60-4
, Pyridine-2-carboxaldehyde 1122-54-9, 4-Acetylpyridine 1126-09-6,
Ethyl isonipecotate 1489-69-6, Cyclopropanecarboxaldehyde 1603-41-4,
2-Amino-5-methylpyridine 1710-98-1, 4-tert-Butylbenzoyl chloride
1776-53-0, 4-Aminocyclohexanecarboxylic acid 1793-07-3,
2-Carbomethoxyphenyl isocyanate 1882-69-5, 5-Methoxy-2-nitrobenzoic acid
2148-56-3, 2-Amino-6-chlorobenzoic acid 2366-70-3,
4,4,4-Trifluorobutan-2-one 2516-95-2, 5-Chloro-2-nitrobenzoic acid
3113-72-2, 5-Methyl-2-nitrobenzoic acid 3678-63-5, 4-Chloro-2-picoline
4315-09-7, 4-Nitroisophthalic acid 4363-93-3, Quinoline-4-carboxaldehyde
4771-47-5, 3-Chloro-2-nitrobenzoic acid 4786-20-3, 2-Butenenitrile
4897-84-1, Methyl 4-bromobutyrate 4920-80-3, 3-Methoxy-2-nitrobenzoic
acid 5350-93-6 5372-81-6, 2-Aminoterephthalic acid dimethyl ester
5428-89-7, 2-Amino-5-chloropyrimidine 5437-38-7, 3-Methyl-2-nitrobenzoic
acid 5469-69-2, 3-Amino-6-chloropyridazine 5470-22-4,
4-Chloropicolinic acid 5538-51-2, Acetylsalicylic acid chloride
6280-88-2, 4-Chloro-2-nitrobenzoic acid 7304-32-7,
2-Fluoro-5-nitrobenzoic acid 7379-35-3, 4-Chloropyridine hydrochloride
7486-35-3, Tributyl(vinyl)tin 10177-29-4, 4-Chloronicotinic acid
10200-59-6, Thiazole-2-carboxaldehyde 14002-51-8, 4-Biphenylcarbonyl
chloride 17012-21-4, Methyl 1-benzylpyrrolidine-3-carboxylate 19235-89
-3, 4-Chloro-2-cyanopyridine 19524-06-2 21717-96-4,
2-Amino-5-fluoropyridine 29943-42-8, Tetrahydro-4H-pyran-4-one 40499-8
3-0, 3-Hydroxypyrrolidine 55737-66-1, 4-Methoxycarbonyl-2-nitrobenzoic
acid 57260-71-6, N-tert-Butoxycarbonylpiperazine 57946-63-1,
2-Bromo-4-trifluoromethylaniline 76143-33-4,
5-Methoxycarbonyl-2-nitrobenzoic acid 79099-07-3,
1-tert-Butoxycarbonyl-4-piperidone 84358-13-4,
1-tert-Butoxycarbonyl-isonipecotic acid 93913-86-1 103057-44-9,
1-tert-Butoxycarbonyl-3-hydroxypyrrolidine 109384-19-2,
1-tert-Butoxycarbonyl-4-hydroxypiperidine 118486-94-5,
2-(Tributylstannyl)furan 124252-41-1, 4-(Tributylstannyl)pyridine
141699-55-0, 1-tert-Butoxycarbonyl-3-hydroxyazetidine 173382-28-0
175278-17-8 183158-31-8 186550-13-0 218777-23-2 219493-02-4
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RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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5470-49-5P 5731-17-9P 17459-03-9P 18229-61-3P 33890-03-8P,
4-Aminoisophthalic acid 61014-96-8P 63069-48-7P,
4-Chloro-2-iodoaniline 70684-84-3P 75541-82-1P 76842-15-4P
97776-06-2P 116721-57-4P 117145-55-8P 117145-66-1P 123855-51-6P,
1-tert-Butoxycarbonyl-4-hydroxymethylpiperidine 130234-74-1P
130309-46-5P 130658-67-2P 137076-22-3P, 1-tert-Butoxycarbonyl-
piperidine-4-carboxaldehyde 138647-49-1P 142374-19-4P 154348-17-1P
159974-55-7P 159974-59-1P 166954-15-0P 168077-29-0P 183170-69-6P
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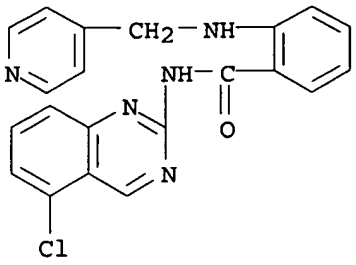
280773-16-2P 280773-17-3P 280773-18-4P 280773-20-8P 280773-21-9P
280773-22-0P 280773-24-2P 280773-25-3P 280773-26-4P 280773-27-5P
280773-28-6P 280773-30-0P 280773-31-1P 280773-32-2P 280773-34-4P
280773-35-5P 280773-36-6P 280773-37-7P 280773-40-2P 280773-42-4P
280773-43-5P 280773-44-6P 280773-46-8P 280773-47-9P 280773-48-0P
280773-49-1P 280773-50-4P 280773-52-6P 280773-53-7P 280773-54-8P
280773-55-9P 280773-57-1P 280773-58-2P 280773-60-6P 280773-61-7P
280773-63-9P 280773-64-0P 280773-66-2P 280773-67-3P 280773-68-4P
280773-69-5P 280773-70-8P 280773-72-0P 280773-73-1P 280773-75-3P
280773-76-4P 280773-78-6P 280773-79-7P 280773-81-1P 280773-82-2P
280773-84-4P 280773-85-5P 280773-86-6P 280773-87-7P 280773-89-9P
280773-90-2P 280773-91-3P 280773-93-5P 280773-94-6P 280773-96-8P
280773-97-9P 280773-98-0P 280773-99-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)
IT 280774-00-7P 280774-01-8P 280774-02-9P 280774-03-0P 280774-04-1P
280774-05-2P 280774-06-3P 280774-07-4P 280774-08-5P 280774-09-6P
280774-15-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Beight Douglas Wade; WO 9900121 A 1999 CAPLUS
(2) Beight Douglas Wade; WO 9900128 A 1999 CAPLUS
(3) Berlex Lab; WO 9628427 A 1996 CAPLUS
(4) Katakura; EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY CHIMICA THERAPEUTICA 1995, V30(5), P387 CAPLUS
(5) Kunitada, S; CURRENT PHARMACEUTICAL DESIGN 1996, V2(5), P6
(6) Schering Ag; WO 9932477 A 1999 CAPLUS

L5 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 267891-53-2 REGISTRY
ED Entered STN: 02 Jun 2000
CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H16 Cl N5 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N	NC5	6	C5N	46.156.30	1
C4N2-C6	NCNC3-C6	6-6	C8N2	591.100.47	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.12	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	6.75	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	45.32	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	116.61	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	136.68	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	122.15	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	55.70	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	10.63	pH 10 25 deg C	(1)
Density (DEN)	1.421+/-0.06 g/cm**3	760 Torr	(1)
Freely Rotatable Bonds (FRB)	4		(1)
H acceptors (HAC)	6		(1)
H donors (HD)	2		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	8		(1)
Koc (KOC)	1.64	pH 1 25 deg C	(1)
Koc (KOC)	3.48	pH 2 25 deg C	(1)
Koc (KOC)	8.07	pH 3 25 deg C	(1)
Koc (KOC)	48.75	pH 4 25 deg C	(1)
Koc (KOC)	327.37	pH 5 25 deg C	(1)
Koc (KOC)	842.43	pH 6 25 deg C	(1)
Koc (KOC)	987.39	pH 7 25 deg C	(1)
Koc (KOC)	882.47	pH 8 25 deg C	(1)
Koc (KOC)	402.41	pH 9 25 deg C	(1)
Koc (KOC)	76.78	pH 10 25 deg C	(1)
logD (LOGD)	0.42	pH 1 25 deg C	(1)
logD (LOGD)	0.74	pH 2 25 deg C	(1)
logD (LOGD)	1.11	pH 3 25 deg C	(1)
logD (LOGD)	1.89	pH 4 25 deg C	(1)
logD (LOGD)	2.72	pH 5 25 deg C	(1)
logD (LOGD)	3.13	pH 6 25 deg C	(1)
logD (LOGD)	3.20	pH 7 25 deg C	(1)
logD (LOGD)	3.15	pH 8 25 deg C	(1)
logD (LOGD)	2.81	pH 9 25 deg C	(1)
logD (LOGD)	2.09	pH 10 25 deg C	(1)
logP (LOGP)	3.463+/-0.615	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.0036 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	3.9 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	1.9 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.78 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.12 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.018 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0070 g/L	pH 6 25 deg C	(1)

Mass Solubility (SLB.MASS)	0.0062 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0070 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.015 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.082 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0062 g/L	Unbuffered Water pH 7.05 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.0000093 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.010 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0048 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0020 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00032 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000047 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000018 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000016 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000018 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000039 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00021 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000016 mol/L	Unbuffered Water pH 7.05 25 deg C	(1)
Molar Volume (MVOL)	274.2+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	389.84		(1)
pKa (PKA)	8.54+/-0.43	Most Acidic 25 deg C	(1) (2)
pKa (PKA)	5.34+/-0.10	Most Basic 25 deg C	(1) (2)
Polar Surface Area (PSA)	79.80 A**2		(1)

This substance may exist in multiple tautomeric forms. The property values in this table are calculated based upon the displayed form and may therefore differ from experimental values based on the actual tautomeric ratio at equilibrium.

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

(2) A significant difference may occur between experimental and calculated values.

See HELP PROPERTIES for information about property data sources in REGISTRY.

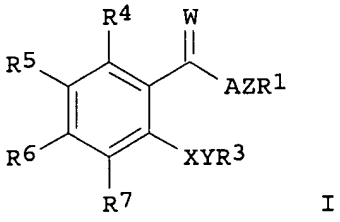
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:334364 CA
TI Preparation of anthranilic acid amides as vascular endothelial growth factor receptor inhibitors.
IN Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz; Bold, Guido; Manley, Paul William; Furet, Pascal; Wood, Jeanette Marjorie; Mestan, Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard; Menrad, Andreas; Schirner, Michael
PA Schering Aktiengesellschaft, Germany; Novartis Aktiengesellschaft
SO PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DT Patent
LA German
IC ICM C07D213-38
ICS C07D409-12; C07D401-12; C07D213-40; C07D413-12; C07D401-12; C07D401-12; C07C237-30; C07D213-61; C07D417-12; C07D401-12; C07D401-12; C07D401-14; C07D401-12; C07D405-12; C07D417-12; C07D405-12; C07D265-26
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000027819	A2	20000518	WO 1999-EP8478	19991109
	WO 2000027819	A3	20000817		
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	DE 19910396	A1	20000907	DE 1999-19910396	19990303
	DE 19910396	C2	20011213		
	CA 2350208	AA	20000518	CA 1999-2350208	19991109
	BR 9915553	A	20010814	BR 1999-15553	19991109
	EP 1129074	A2	20010905	EP 1999-953967	19991109
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	TR 200101307	T2	20020521	TR 2001-20010130	19991109
	JP 2002529452	T2	20020910	JP 2000-580999	19991109
	EE 200100258	A	20021216	EE 2001-258	19991109
	NZ 511413	A	20040130	NZ 1999-511413	19991109
	AU 771180	B2	20040318	AU 2000-10454	19991109
	NO 2001002245	A	20010710	NO 2001-2245	20010507
	BG 105588	A	20020430	BG 2001-105588	20010611
	HK 1041882	A1	20050318	HK 2002-103628	20020514
PRAI	GB 1998-24579	19981110			
	DE 1999-19910396	19990303			
	WO 1999-EP8478	19991109			

GI



I

AB Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q, alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl, 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl; R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo, (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H, alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (preparation given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl)anthranilamide. The latter inhibited VEGFR I with IC50 = 0.05 μM.

ST anthranilamide prepn VEGF receptor inhibitor; angiogenesis inhibitor anthranilamide; vascular endothelial growth factor receptor inhibitor prepn anthranilamide

IT Blood vessel, neoplasm
(angiofibroma, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Medical goods
(catheters, antithrombogenic; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Kidney, disease
(diabetic nephropathy, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Vascular endothelial growth factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(gene KDR, inhibitors; preparation of anthranilic acid amides as VEGF

receptor inhibitors)
IT Vascular endothelial growth factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(gene flt 1, inhibitors; preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT Kidney, disease
(glomerulonephritis, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT Blood vessel, neoplasm
(hemangioma, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT Nerve, disease
(injury, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT Blood vessel, disease
(microangiopathy, treatment of thrombotic microangiopathy; preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT Kidney, disease
(nephrosclerosis, treatment of malignant nephrosclerosis; preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT Angiogenesis inhibitors
Antiarteriosclerotics
Antiarthritics
Antitumor agents
(preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT Medical goods
(stents, opening maintenance; preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT Cirrhosis
Eye, disease
Kidney, disease
Psoriasis
Transplant rejection
(treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT 267891-62-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT 267891-04-3P 267891-05-4P 267891-06-5P 267891-07-6P 267891-08-7P
267891-09-8P 267891-10-1P 267891-11-2P 267891-12-3P 267891-13-4P
267891-14-5P 267891-15-6P 267891-16-7P 267891-17-8P 267891-18-9P
267891-19-0P 267891-20-3P 267891-21-4P 267891-22-5P 267891-23-6P
267891-24-7P 267891-25-8P 267891-26-9P 267891-27-0P 267891-28-1P
267891-29-2P 267891-30-5P 267891-31-6P 267891-32-7P 267891-33-8P
267891-34-9P 267891-35-0P 267891-36-1P 267891-37-2P 267891-38-3P
267891-39-4P 267891-40-7P 267891-41-8P 267891-42-9P 267891-43-0P
267891-44-1P 267891-45-2P 267891-46-3P 267891-47-4P 267891-48-5P
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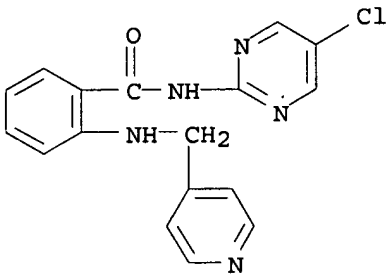
267891-70-3P 267891-72-5P 267891-73-6P 267891-74-7P 267891-75-8P
267891-76-9P 267891-77-0P 267891-78-1P 267891-79-2P 267891-80-5P
267891-81-6P 267891-82-7P 267891-83-8P 267891-84-9P 267891-85-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT 267891-91-8 267891-92-9 267891-93-0 267891-94-1 267891-95-2
267891-96-3 267891-97-4 267891-98-5 267891-99-6 267892-00-2
267892-01-3 267892-02-4 267892-03-5 267892-04-6 267892-05-7
267892-06-8 267892-07-9 267892-09-1 267892-11-5 267892-12-6
267892-13-7 267892-14-8 267892-15-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT 104-86-9, 4-Chlorobenzylamine 118-48-9, Isatoic anhydride 123-11-5, 4-Methoxybenzaldehyde, reactions 134-20-3, Methyl anthranilate 582-22-9, 2-Phenylpropylamine 635-21-2, 5-Chloroanthranilic acid 872-85-5, Pyridine-4-carboxaldehyde 19335-11-6, 5-Aminoindazole 101066-61-9, 2-Chloro-4-pyridinecarboxaldehyde 267891-89-4 267891-90-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)
IT 16512-74-6P 267891-86-1P 267891-87-2P 267891-88-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

L5 ANSWER 5 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 267891-24-7 REGISTRY
ED Entered STN: 02 Jun 2000
CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H14 Cl N5 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	1
C5N	NC5	6	C5N	46.156.30	1
C4N2	NCNC3	6	C4N2	46.195.39	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	1.0	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	6.52	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	16.71	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	19.82	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	20.02	pH 8 25 deg C	(1)

Bioconc. Factor (BCF)	18.47	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	10.34	pH 10 25 deg C	(1)
Density (DEN)	1.415+/-0.06 g/cm**3	760 Torr	(1)
Freely Rotatable Bonds (FRB)	4		(1)
H acceptors (HAC)	6		(1)
H donors (HD)	2		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	8		(1)
Koc (KOC)	1.0	pH 1 25 deg C	(1)
Koc (KOC)	1.05	pH 2 25 deg C	(1)
Koc (KOC)	2.34	pH 3 25 deg C	(1)
Koc (KOC)	14.35	pH 4 25 deg C	(1)
Koc (KOC)	96.41	pH 5 25 deg C	(1)
Koc (KOC)	247.20	pH 6 25 deg C	(1)
Koc (KOC)	293.14	pH 7 25 deg C	(1)
Koc (KOC)	296.15	pH 8 25 deg C	(1)
Koc (KOC)	273.17	pH 9 25 deg C	(1)
Koc (KOC)	152.97	pH 10 25 deg C	(1)
logD (LOGD)	-0.60	pH 1 25 deg C	(1)
logD (LOGD)	-0.43	pH 2 25 deg C	(1)
logD (LOGD)	-0.09	pH 3 25 deg C	(1)
logD (LOGD)	0.70	pH 4 25 deg C	(1)
logD (LOGD)	1.53	pH 5 25 deg C	(1)
logD (LOGD)	1.94	pH 6 25 deg C	(1)
logD (LOGD)	2.01	pH 7 25 deg C	(1)
logD (LOGD)	2.02	pH 8 25 deg C	(1)
logD (LOGD)	1.98	pH 9 25 deg C	(1)
logD (LOGD)	1.73	pH 10 25 deg C	(1)
logP (LOGP)	2.022+/-0.612	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.054 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	23 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	16 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	7.1 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	1.2 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.17 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.068 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.058 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.054 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.061 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.11 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.054 g/L	Unbuffered Water pH 7.57 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.00016 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.069 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.046 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.021 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0034 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00050 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00020 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00017 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00016 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00018 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00032 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00016 mol/L	Unbuffered Water pH 7.57 25 deg C	(1)
Molar Volume (MVOL)	240.0+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	339.78		(1)
pKa (PKA)	10.01+/-0.70	Most Acidic 25 deg C	(1)
pKa (PKA)	5.33+/-0.10	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	79.80 A**2		(1)

This substance may exist in multiple tautomeric forms. The property values in

this table are calculated based upon the displayed form and may therefore differ from experimental values based on the actual tautomeric ratio at equilibrium.

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

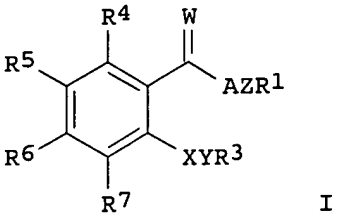
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 132:334364 CA
TI Preparation of anthranilic acid amides as vascular endothelial growth factor receptor inhibitors.
IN Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz; Bold, Guido; Manley, Paul William; Furet, Pascal; Wood, Jeanette Marjorie; Mestan, Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard; Menrad, Andreas; Schirner, Michael
PA Schering Aktiengesellschaft, Germany; Novartis Aktiengesellschaft
SO PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DT Patent
LA German
IC ICM C07D213-38
ICS C07D409-12; C07D401-12; C07D213-40; C07D413-12; C07D401-12; C07D401-12; C07C237-30; C07D213-61; C07D417-12; C07D401-12; C07D401-12; C07D401-14; C07D401-12; C07D405-12; C07D417-12; C07D405-12; C07D265-26
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000027819	A2	20000518	WO 1999-EP8478	19991109
	WO 2000027819	A3	20000817		
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	DE 19910396	A1	20000907	DE 1999-19910396	19990303
	DE 19910396	C2	20011213		
	CA 2350208	AA	20000518	CA 1999-2350208	19991109
	BR 9915553	A	20010814	BR 1999-15553	19991109
	EP 1129074	A2	20010905	EP 1999-953967	19991109
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	TR 200101307	T2	20020521	TR 2001-20010130	19991109
	JP 2002529452	T2	20020910	JP 2000-580999	19991109
	EE 200100258	A	20021216	EE 2001-258	19991109
	NZ 511413	A	20040130	NZ 1999-511413	19991109
	AU 771180	B2	20040318	AU 2000-10454	19991109
	NO 2001002245	A	20010710	NO 2001-2245	20010507
	BG 105588	A	20020430	BG 2001-105588	20010611
	HK 1041882	A1	20050318	HK 2002-103628	20020514
PRAI	GB 1998-24579	19981110			
	DE 1999-19910396	19990303			
	WO 1999-EP8478	19991109			

GI



I

AB Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q, alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl, 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl; R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo, (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H, alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (preparation given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl)anthranilamide. The latter inhibited VEGFR I with IC50 = 0.05 μM.

ST anthranilamide prepn VEGF receptor inhibitor; angiogenesis inhibitor anthranilamide; vascular endothelial growth factor receptor inhibitor prepn anthranilamide

IT Blood vessel, neoplasm
(angiofibroma, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Medical goods
(catheters, antithrombogenic; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Kidney, disease
(diabetic nephropathy, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Vascular endothelial growth factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(gene KDR, inhibitors; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Vascular endothelial growth factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(gene flt 1, inhibitors; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Kidney, disease
(glomerulonephritis, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Blood vessel, neoplasm
(hemangioma, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Nerve, disease
(injury, treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Blood vessel, disease
(microangiopathy, treatment of thrombotic microangiopathy; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Kidney, disease
(nephrosclerosis, treatment of malignant nephrosclerosis; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Angiogenesis inhibitors
Antiarteriosclerotics
Antiarthritics
Antitumor agents
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Medical goods
(stents, opening maintenance; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT Cirrhosis
Eye, disease
Kidney, disease
Psoriasis

Transplant rejection
(treatment; preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT 267891-62-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT 267891-04-3P 267891-05-4P 267891-06-5P 267891-07-6P 267891-08-7P
267891-09-8P 267891-10-1P 267891-11-2P 267891-12-3P 267891-13-4P
267891-14-5P 267891-15-6P 267891-16-7P 267891-17-8P 267891-18-9P
267891-19-0P 267891-20-3P 267891-21-4P 267891-22-5P 267891-23-6P
267891-24-7P 267891-25-8P 267891-26-9P 267891-27-0P 267891-28-1P
267891-29-2P 267891-30-5P 267891-31-6P 267891-32-7P 267891-33-8P
267891-34-9P 267891-35-0P 267891-36-1P 267891-37-2P 267891-38-3P
267891-39-4P 267891-40-7P 267891-41-8P 267891-42-9P 267891-43-0P
267891-44-1P 267891-45-2P 267891-46-3P 267891-47-4P 267891-48-5P
267891-49-6P 267891-50-9P 267891-51-0P 267891-52-1P 267891-53-2P
267891-54-3P 267891-55-4P 267891-56-5P 267891-57-6P 267891-58-7P
267891-59-8P 267891-60-1P 267891-61-2P 267891-63-4P 267891-64-5P
267891-65-6P 267891-66-7P 267891-67-8P 267891-68-9P 267891-69-0P
267891-70-3P 267891-72-5P 267891-73-6P 267891-74-7P 267891-75-8P
267891-76-9P 267891-77-0P 267891-78-1P 267891-79-2P 267891-80-5P
267891-81-6P 267891-82-7P 267891-83-8P 267891-84-9P 267891-85-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT 267891-91-8 267891-92-9 267891-93-0 267891-94-1 267891-95-2
267891-96-3 267891-97-4 267891-98-5 267891-99-6 267892-00-2
267892-01-3 267892-02-4 267892-03-5 267892-04-6 267892-05-7
267892-06-8 267892-07-9 267892-09-1 267892-11-5 267892-12-6
267892-13-7 267892-14-8 267892-15-9
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

IT 104-86-9, 4-Chlorobenzylamine 118-48-9, Isatoic anhydride 123-11-5, 4-Methoxybenzaldehyde, reactions 134-20-3, Methyl anthranilate 582-22-9, 2-Phenylpropylamine 635-21-2, 5-Chloroanthranilic acid 872-85-5, Pyridine-4-carboxaldehyde 19335-11-6, 5-Aminoindazole 101066-61-9, 2-Chloro-4-pyridinecarboxaldehyde 267891-89-4 267891-90-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

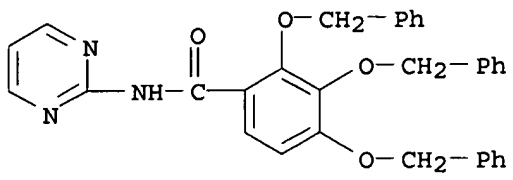
IT 16512-74-6P 267891-86-1P 267891-87-2P 267891-88-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

L5 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 180206-29-5 REGISTRY
ED Entered STN: 29 Aug 1996
CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C32 H27 N3 O4
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	4

C4N2 |NCNC3 |6 |C4N2 |46.195.39 |1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	8607.26	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	10515.24	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	10753.82	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	10778.27	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	10780.63	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	10780.01	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	10771.36	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	10685.44	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	9896.65	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	5715.35	pH 10 25 deg C	(1)
Density (DEN)	1.265+/-0.06 g/cm**3	760 Torr	(1)
Freely Rotatable Bonds (FRB)	10		(1)
H acceptors (HAC)	7		(1)
H donors (HD)	1		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	8		(1)
Koc (KOC)	21384.27	pH 1 25 deg C	(1)
Koc (KOC)	26124.53	pH 2 25 deg C	(1)
Koc (KOC)	26717.24	pH 3 25 deg C	(1)
Koc (KOC)	26777.98	pH 4 25 deg C	(1)
Koc (KOC)	26783.86	pH 5 25 deg C	(1)
Koc (KOC)	26782.33	pH 6 25 deg C	(1)
Koc (KOC)	26760.84	pH 7 25 deg C	(1)
Koc (KOC)	26547.35	pH 8 25 deg C	(1)
Koc (KOC)	24587.68	pH 9 25 deg C	(1)
Koc (KOC)	14199.46	pH 10 25 deg C	(1)
logD (LOGD)	5.51	pH 1 25 deg C	(1)
logD (LOGD)	5.60	pH 2 25 deg C	(1)
logD (LOGD)	5.61	pH 3 25 deg C	(1)
logD (LOGD)	5.61	pH 4 25 deg C	(1)
logD (LOGD)	5.61	pH 5 25 deg C	(1)
logD (LOGD)	5.61	pH 6 25 deg C	(1)
logD (LOGD)	5.61	pH 7 25 deg C	(1)
logD (LOGD)	5.60	pH 8 25 deg C	(1)
logD (LOGD)	5.57	pH 9 25 deg C	(1)
logD (LOGD)	5.33	pH 10 25 deg C	(1)
logP (LOGP)	5.610+/-0.611	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.00016 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00020 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00017 g/L	pH 9 25 deg C	(1)

Mass Solubility (SLB.MASS)	0.00030 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.00016 g/L	Unbuffered Water pH 7.00 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.00000031 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000038 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000033 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000058 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00000031 mol/L	Unbuffered Water pH 7.00 25 deg C	(1)
Molar Volume (MVOL)	408.8+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	517.57		(1)
pKa (PKA)	10.04+/-0.70	Most Acidic 25 deg C	(1)
pKa (PKA)	0.40+/-0.33	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	82.57 A**2		(1)

This substance may exist in multiple tautomeric forms. The property values in this table are calculated based upon the displayed form and may therefore differ from experimental values based on the actual tautomeric ratio at equilibrium.

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

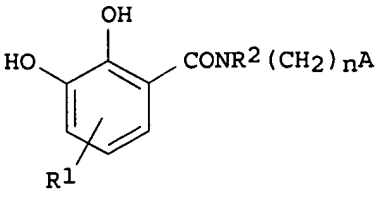
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 125:167581 CA
TI Preparation of hydroxybenzamide derivatives as prevention and treatment agents for bone diseases
IN Nomoto, Takashi; Kawakami, Kumiko; Akagawa, Akiko; Matsuyama, Kenji; Torigoe, Koichiro
PA Banyu Pharma Co Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C07C235-64
ICS A61K031-165; A61K031-415; A61K031-44; A61K031-445; A61K031-47; A61K031-505; C07C235-56; C07C237-42; C07C255-24; C07D211-06; C07D211-22; C07D211-58; C07D213-75; C07D217-06; C07D231-56; C07D233-88; C07D239-26; C07D295-18
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08143525	A2	19960604	JP 1994-311235	19941121

PRAI JP 1994-311235 19941121
GI



I

AB The title bone disease inhibitors contain a compound (I) [R1 = H, halo, OH, NO2, lower alkyl, lower alkoxy; R2 = H, lower alkyl; n = 0-3; A = aryl, heteroaryl; A and R2 may combine to complete piperidine or tetrahydroisoquinoline ring]. I is an efficient component for prevention and treatment of bone diseases caused by Vacuolar ATPase. Thus, 2,3,4-tribenzyloxybenzoic acid was reacted with aniline in the presence of 4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide, followed by hydrogenation to give I [R1 = OH; R2 = H; n = 0; A = Ph], 4 μM of which showed Vacuolar ATPase inhibiting activity of 97%.

ST hydroxybenzamide prepn prevention treatment bone disease; Vacuolar ATPase inhibitor hydroxybenzamide

IT Bone, disease
(synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)

IT 9000-83-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(proton-translocating; synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)

IT 180206-07-9P 180206-26-2P 180206-27-3P 180206-28-4P 180206-29-5P 180206-30-8P 180206-33-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)

IT 180205-89-4P 180205-90-7P 180205-91-8P 180205-92-9P 180205-93-0P 180205-94-1P 180205-95-2P 180205-96-3P 180205-97-4P 180205-98-5P 180205-99-6P 180206-00-2P 180206-01-3P 180206-02-4P 180206-03-5P 180206-04-6P 180206-05-7P 180206-06-8P 180206-08-0P 180206-09-1P 180206-10-4P 180206-11-5P 180206-12-6P 180206-13-7P 180206-14-8P 180206-15-9P 180206-16-0P 180206-17-1P 180206-18-2P 180206-19-3P 180206-20-6P 180206-21-7P 180206-22-8P 180206-23-9P 180206-24-0P 180206-25-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)

IT 62-53-3, Aniline, reactions 88-74-4, o-Nitroaniline 100-44-7, Benzyl chloride, reactions 106-50-3, 1,4-Phenylenediamine, reactions 543-27-1, Isobutyl chloroformate 573-11-5, 2,3,4-Trimethoxybenzoic acid 610-02-6, 2,3,4-Trihydroxybenzoic acid 1122-58-3, 4-Dimethylaminopyridine 10294-33-4, Boron tribromide 25952-53-8, 1-Ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride 28675-03-8, Dimethylaminoaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)

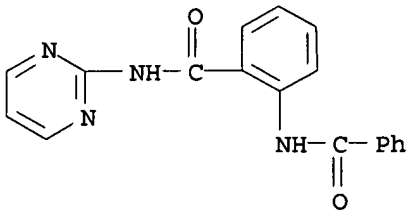
IT 180206-31-9P 180206-32-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)

L5 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 69589-68-0 REGISTRY
ED Entered STN: 16 Nov 1984
CN Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H14 N4 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)
DT.CA CAplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C6	C6	6	C6	46.150.18	2
C4N2	NCNC3	6	C4N2	46.195.39	1



Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	29.12	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	38.52	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	39.80	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	39.94	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	39.95	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	39.95	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	39.94	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	39.81	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	38.59	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	29.56	pH 10 25 deg C	(1)
Density (DEN)	1.362+/-0.06 g/cm**3	760 Torr	(1)
Freely Rotatable Bonds (FRB)	3		(1)
H acceptors (HAC)	6		(1)
H donors (HD)	2		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	8		(1)
Koc (KOC)	355.13	pH 1 25 deg C	(1)
Koc (KOC)	469.73	pH 2 25 deg C	(1)
Koc (KOC)	485.40	pH 3 25 deg C	(1)
Koc (KOC)	487.02	pH 4 25 deg C	(1)
Koc (KOC)	487.18	pH 5 25 deg C	(1)
Koc (KOC)	487.18	pH 6 25 deg C	(1)
Koc (KOC)	487.03	pH 7 25 deg C	(1)
Koc (KOC)	485.49	pH 8 25 deg C	(1)
Koc (KOC)	470.63	pH 9 25 deg C	(1)
Koc (KOC)	360.54	pH 10 25 deg C	(1)
logD (LOGD)	2.27	pH 1 25 deg C	(1)
logD (LOGD)	2.39	pH 2 25 deg C	(1)
logD (LOGD)	2.41	pH 3 25 deg C	(1)
logD (LOGD)	2.41	pH 4 25 deg C	(1)
logD (LOGD)	2.41	pH 5 25 deg C	(1)
logD (LOGD)	2.41	pH 6 25 deg C	(1)
logD (LOGD)	2.41	pH 7 25 deg C	(1)
logD (LOGD)	2.41	pH 8 25 deg C	(1)
logD (LOGD)	2.39	pH 9 25 deg C	(1)
logD (LOGD)	2.28	pH 10 25 deg C	(1)
logP (LOGP)	2.410+/-0.630	25 deg C	(1)

Mass Intrinsic Solubility (ISLB.MASS)	0.020 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	0.028 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.021 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.021 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.027 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.020 g/L	Unbuffered Water pH 6.96 25 deg C	(1)
Molar Intrinsic Solubility (ISLB.MOL)	0.000064 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000088 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000066 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000066 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000086 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000064 mol/L	Unbuffered Water pH 6.96 25 deg C	(1)
Molar Volume (MVOL)	233.6+/-3.0 cm**3/mol	20 deg C 760 Torr	(1)
Molecular Weight (MW)	318.33		(1)
pKa (PKA)	10.45+/-0.70	Most Acidic 25 deg C	(1)
pKa (PKA)	0.57+/-0.33	Most Basic 25 deg C	(1)
Polar Surface Area (PSA)	83.98 A**2		(1)

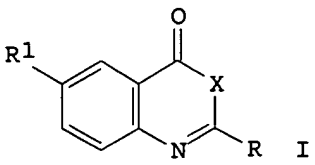
(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.14 ((C) 1994-2006 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 90:121516 CA
TI Condensation of acetanthranil and phenylanthranil with certain aminoheterocycles. Attempted preparation of some 2,3-disubstituted 4(3H)-quinazolinones
AU El-Zanfally, S.
CS Fac. Pharm., Cairo Univ., Cairo, Egypt
SO Egyptian Journal of Pharmaceutical Sciences (1978), Volume Date 1976, 17(1), 29-34
CODEN: EJPSBZ; ISSN: 0301-5068
DT Journal
LA English
CC 28-14 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 25
GI



I

AB Treating 2-methyl-4H-3,1-benzoxazin-4-ones (I; X = O; R = Me; R1 = H, Br) with amines R2NH2 (R2 = 2-pyridyl, 4-antipyrinyl) yielded 35-81% the corresponding quinazolinones (I; X = NR2). The reactions were carried out by fusing the reactants at 150-60° for 3 h or by refluxing in pyridine-dioxane for 2 h. Similar reaction of I (X = O, R = Ph, R1 = H) with R2NH2 (R2 = 2-, 3-, or 4-pyridyl; 2-pyrimidinyl, or 4-antipyrinyl) gave o-R2NHCOC6H4NHCOPh.

ST quinazolinone methyl; benzoxazinone methyl condensation pyridylamine; antipyrinylamine condensation benzoxazinone

IT 109-12-6 462-08-8 504-24-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with 2-phenyl-3,1-benzoxazin-4-one)

IT 83-07-8 504-29-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with 3,1-benzoxazin-4-one)

IT 19165-25-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with antipyrinylamine)

IT 525-76-8 1022-46-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with pyridyl- or antipyrinylamine)

IT 890-03-9P 1898-05-1P 69589-64-6P 69589-65-7P 69589-66-8P
69589-67-9P 69589-68-0P 69608-79-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

=> d his

(FILE 'HOME' ENTERED AT 14:36:32 ON 14 FEB 2006)

FILE 'REGISTRY' ENTERED AT 14:37:27 ON 14 FEB 2006
L1 STRUCTURE UPLOADED
L2 0 S L1

FILE 'CAPLUS' ENTERED AT 14:38:12 ON 14 FEB 2006
S L1

FILE 'REGISTRY' ENTERED AT 14:38:17 ON 14 FEB 2006
L3 0 S L1

FILE 'CAPLUS' ENTERED AT 14:38:17 ON 14 FEB 2006
L4 0 S L3
S L1

FILE 'REGISTRY' ENTERED AT 14:38:44 ON 14 FEB 2006
L5 7 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:38:50 ON 14 FEB 2006
L6 5 S L5 FULL

FILE 'REGISTRY' ENTERED AT 14:39:15 ON 14 FEB 2006

FILE 'CAPLUS' ENTERED AT 14:39:17 ON 14 FEB 2006
S L1 FULL 2

FILE 'REGISTRY' ENTERED AT 14:39:39 ON 14 FEB 2006
L7 0 S L1

FILE 'CAPLUS' ENTERED AT 14:39:40 ON 14 FEB 2006

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L8             0 S L7

      FILE 'REGISTRY' ENTERED AT 14:40:42 ON 14 FEB 2006

      FILE 'CAPLUS' ENTERED AT 14:40:54 ON 14 FEB 2006

      FILE 'REGISTRY' ENTERED AT 14:41:09 ON 14 FEB 2006

      FILE 'CAPLUS' ENTERED AT 14:41:13 ON 14 FEB 2006

=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:h
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.46     236.75

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -4.97

 SESSION WILL BE HELD FOR 60 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:41:32 ON 14 FEB 2006
Connection closed by remote host
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G1:O,N

G2:O,[*1],[*2]

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:CLASS 19:CLASS 20:Atom 21:Atom 22:CLASS

L1 STRUCTURE UPLOADED

=> s l1 sub sam
ENTER SUBSET L# OR (END):l1
L1 MAY NOT BE USED HERE
The L-number must have been created by a search in this file. To see
all L-numbers defined in this session, enter DISPLAY HISTORY at an
arrow prompt (=>). For additional information on subset searching in
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ENTER SUBSET L# OR (END):end
SEARCH ENDED BY USER

=> s l1
SAMPLE SEARCH INITIATED 14:10:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 106 TO 614
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.88 1.09

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FILE COVERS 1907 - 14 Feb 2006 VOL 144 ISS 8
FILE LAST UPDATED: 13 Feb 2006 (20060213/ED)

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http://www.cas.org/infopolicy.html

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REGlstRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:11:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 106 TO 614
PROJECTED ANSWERS: 0 TO 0

L3 0 SEA SSS SAM L1

L4 0 L3

=> s l1
REGIstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:12:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 18 TO ITERATE

100.0% PROCESSED 18 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 106 TO 614
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L1

L6 0 L5

=> s l1 full
REGIstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 14:12:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 340 TO ITERATE

100.0% PROCESSED 340 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

L7 7 SEA SSS FUL L1

L8 5 L7

=> d 1

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:457059 CAPLUS
DN 133:89437
TI Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors
IN Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PA Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SO PCT Int. Appl., 403 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000039118	A1	20000706	WO 1999-US29946	19991215
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2361149	AA	20000706	CA 1999-2361149	19991215
	EP 1140903	A1	20011010	EP 1999-964279	19991215
	EP 1140903	B1	20040804		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2002533454	T2	20021008	JP 2000-591029	19991215
	AT 272633	E	20040815	AT 1999-964279	19991215
	ES 2226485	T3	20050316	ES 1999-964279	19991215
	US 6635657	B1	20031021	US 2001-857751	20010608
	US 2004029874	A1	20040212	US 2003-629760	20030729
	US 6759414	B2	20040706		
	US 2005282862	A1	20051222	US 2003-629817	20030729
PRAI	US 1998-113556P	P	19981223		
	WO 1999-US29946	W	19991215		
	US 2001-857751	A3	20010608		

OS MARPAT 133:89437
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d iall 1

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:457059 CAPLUS
DOCUMENT NUMBER: 133:89437
ENTRY DATE: Entered STN: 07 Jul 2000
TITLE: Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors
INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong

PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SOURCE: PCT Int. Appl., 403 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
INT. PATENT CLASSIF.:
MAIN: C07D401-14
SECONDARY: C07D401-12; C07D417-14; C07D409-14; C07D405-14; C07D213-74; A61K031-395; A61K031-435; A61K031-495; A61P007-02; C07D401-14; C07D213-00; C07D213-00; C07D211-00
CLASSIFICATION: 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 28, 63
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000039118	A1	20000706	WO 1999-US29946		19991215
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2361149	AA	20000706	CA 1999-2361149		19991215
EP 1140903	A1	20011010	EP 1999-964279		19991215
EP 1140903	B1	20040804			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2002533454	T2	20021008	JP 2000-591029		19991215
AT 272633	E	20040815	AT 1999-964279		19991215
ES 2226485	T3	20050316	ES 1999-964279		19991215
US 6635657	B1	20031021	US 2001-857751		20010608
US 2004029874	A1	20040212	US 2003-629760		20030729
US 6759414	B2	20040706			
US 2005282862	A1	20051222	US 2003-629817		20030729
PRIORITY APPLN. INFO.:			US 1998-113556P	P	19981223
			WO 1999-US29946	W	19991215
			US 2001-857751	A3	20010608

PATENT CLASSIFICATION CODES:

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2000039118	ICM	C07D401-14
	ICS	C07D401-12; C07D417-14; C07D409-14; C07D405-14; C07D213-74; A61K031-395; A61K031-435; A61K031-495; A61P007-02; C07D401-14; C07D213-00; C07D213-00; C07D211-00
	IPCI	C07D0401-14 [ICM,7]; C07D0401-12 [ICS,7]; C07D0417-14 [ICS,7]; C07D0409-14 [ICS,7]; C07D0405-14 [ICS,7]; C07D0213-74 [ICS,7]; A61K0031-395 [ICS,7]; A61K0031-435 [ICS,7]; A61K0031-495 [ICS,7]; A61P0007-02 [ICS,7]; C07D0401-14 [ICS,7]; C07D0213-00 [ICS,7]; C07D0211-00 [ICS,7]
	ECLA	C07D213/75B8; C07D409/14+335+213+211; C07D417/14+277B+213+211; C07D401/12+213+205; C07D401/12+213+211; C07D401/12+213+207; C07D401/12+237B+211; C07D401/14+213+211+211; C07D401/14+213+211+205; C07D401/14+215+213+211; C07D401/14+213+213+207; C07D401/14+213+213+211; C07D401/14+233+213+211; C07D401/14+237B+213+211; C07D401/14+239B+213+211; C07D405/14+309+213+211; C07D405/14+307B+213+211; C07D409/14+333B+213+211
CA 2361149	IPCI	C07D0401-14 [ICM,7]; C07D0211-00 [ICS,7]; C07D0213-00 [ICS,7]; A61P0007-02 [ICS,7]; C07D0401-12 [ICS,7]; C07D0405-14 [ICS,7]; C07D0409-14 [ICS,7]; C07D0417-14 [ICS,7]; A61K0031-395 [ICS,7]; A61K0031-435 [ICS,7]; A61K0031-495 [ICS,7]; C07D0213-74 [ICS,7]

EP 1140903	IPCI	C07D0401-14 [ICM,6]; C07D0401-12 [ICS,6]; C07D0417-14 [ICS,6]; C07D0409-14 [ICS,6]; C07D0405-14 [ICS,6]; C07D0213-74 [ICS,6]; A61K0031-395 [ICS,6]; A61K0031-435 [ICS,6]; A61K0031-495 [ICS,6]; A61P0007-02 [ICS,6]; C07D0401-14 [ICI,6]; C07D0213-00 [ICI,6]; C07D0211-00 [ICI,6]
JP 2002533454	IPCI	C07D0213-75 [ICM,7]; A61K0031-44 [ICS,7]; A61K0031-4427 [ICS,7]; A61K0031-4439 [ICS,7]; A61K0031-444 [ICS,7]; A61K0031-4545 [ICS,7]; A61K0031-4709 [ICS,7]; A61K0031-496 [ICS,7]; A61K0031-501 [ICS,7]; A61K0031-506 [ICS,7]; A61K0031-5377 [ICS,7]; A61P0007-02 [ICS,7]; A61P0009-10 [ICS,7]; C07D0401-12 [ICS,7]; C07D0401-14 [ICS,7]; C07D0405-14 [ICS,7]; C07D0407-14 [ICS,7]; C07D0409-14 [ICS,7]; C07D0417-14 [ICS,7]
AT 272633	IPCI	C07D0401-14 [ICM,7]; C07D0401-12 [ICS,7]; C07D0417-14 [ICS,7]; C07D0409-14 [ICS,7]; C07D0405-14 [ICS,7]; C07D0213-74 [ICS,7]; A61K0031-395 [ICS,7]; A61K0031-435 [ICS,7]
ES 2226485	IPCI	C07D0401-14 [ICM,7]; C07D0401-12 [ICS,7]; C07D0417-14 [ICS,7]; C07D0409-14 [ICS,7]; C07D0405-14 [ICS,7]; C07D0213-74 [ICS,7]; A61K0031-395 [ICS,7]; A61K0031-435 [ICS,7]; A61K0031-495 [ICS,7]; A61P0007-02 [ICS,7]; C07D0213-00 [ICS,7]; C07D0211-00 [ICS,7]
US 6635657	IPCI	A61K0031-4545 [ICM,7]; A61K0031-495 [ICS,7]; C07D0401-12 [ICS,7]; C07D0401-14 [ICS,7]; C07D0409-14 [ICS,7]; A61P0007-02 [ICS,7]
	IPCR	C07D0213-00 [I,C]; C07D0213-75 [I,A]; C07D0401-00 [I,C]; C07D0401-12 [I,A]; C07D0401-14 [I,A]; C07D0405-00 [I,C]; C07D0405-14 [I,A]; C07D0409-00 [I,C]; C07D0409-14 [I,A]; C07D0417-00 [I,C]; C07D0417-14 [I,A]
	NCL	514/318.000; 514/235.500; 514/237.200; 514/252.030; 514/253.010; 514/275.000; 514/314.000; 514/332.000; 514/333.000; 514/340.000; 514/343.000; 514/352.000; 544/130.000; 544/238.000; 544/331.000; 544/361.000; 544/364.000; 546/175.000; 546/194.000; 546/256.000; 546/262.000; 546/268.100; 546/278.400; 546/309.000
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US 2004029874	IPCI	A61K0031-54 [ICM,7]; A61K0031-537 [ICS,7]; A61K0031-495 [ICS,7]; A61K0031-445 [ICS,7]; A61K0031-426 [ICS,7]; A61K0031-421 [ICS,7]; A61K0031-4164 [ICS,7]; A61K0031-277 [ICS,7]
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US 2005282862	IPCI	A61K0031-4545 [ICM,7]; A61K0031-4439 [ICS,7]; C07D0041-02 [ICS,7]
	NCL	514/318.000; 514/326.000; 546/194.000; 546/207.000
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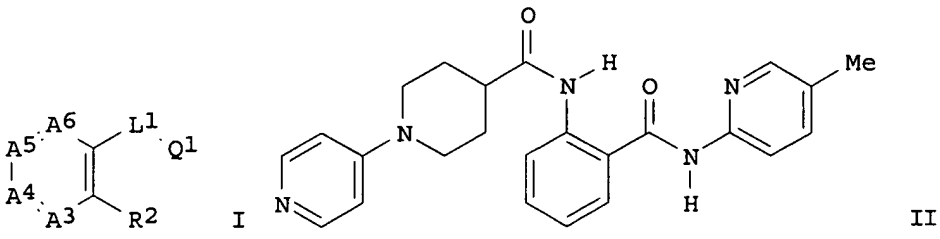
C07D401/12+213+211; C07D401/12+237B+211;
C07D401/14+213+211+205; C07D401/14+213+211+211;
C07D401/14+213+213+207; C07D401/14+213+213+211;
C07D401/14+215+213+211; C07D401/14+233+213+211;
C07D401/14+237B+213+211; C07D401/14+239B+213+211;
C07D405/14+307B+213+211; C07D405/14+309+213+211;
C07D409/14+333B+213+211; C07D409/14+335+213+211;
C07D417/14+277B+213+211

OTHER SOURCE(S): MARPAT 133:89437

GRAPHIC IMAGE:



ABSTRACT:
The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

SUPPL. TERM: arom amide heteroaryl prepn formulation factor Xa inhibitor anticoagulant

INDEX TERM: Anticoagulants
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

INDEX TERM: 280769-11-1P 280769-16-6P 280769-22-4P 280769-23-5P
280769-24-6P 280769-46-2P 280769-59-7P 280769-68-8P
280769-83-7P 280770-51-6P 280770-52-7P 280770-59-4P
280770-66-3P 280770-79-8P 280770-91-4P 280770-93-6P
280770-95-8P 280771-19-9P 280771-47-3P 280771-49-5P
280771-53-1P 280771-55-3P
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

INDEX TERM: 280768-65-2P 280768-66-3P 280768-67-4P 280768-68-5P
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(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

INDEX TERM: 280771-27-9P 280771-28-0P 280771-29-1P 280771-30-4P
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280771-48-4P 280771-50-8P 280771-51-9P 280771-52-0P
280771-54-2P 280771-56-4P 280771-57-5P
ROLE: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

INDEX TERM: 9002-05-5, Factor Xa
ROLE: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

INDEX TERM: 67-64-1, Acetone, reactions 75-64-9, tert-Butylamine, reactions 78-84-2, Isobutyraldehyde 78-93-3, Methylethyl ketone, reactions 89-98-5, 2-Chlorobenzaldehyde 96-22-0,

3-Pentanone 96-33-3 97-96-1, 2-Ethylbutyraldehyde 98-01-1, Furan-2-carboxaldehyde, reactions 98-74-8, 4-Nitrobenzenesulfonyl chloride 98-80-6, Phenylboronic acid 99-88-7, 4-Isopropylaniline 99-92-3 100-52-7, Benzaldehyde, reactions 104-88-1, 4-Chlorobenzaldehyde, reactions 105-36-2, Ethyl bromoacetate 105-58-8, Diethyl carbonate 106-47-8, 4-Chloroaniline, reactions 107-13-1, 2-Propenenitrile, reactions 108-94-1, Cyclohexanone, reactions 110-52-1, 1,4-Dibromobutane 111-42-2, reactions 120-92-3, Cyclopentanone 122-85-0, 4-Acetamidobenzaldehyde 123-11-5, 4-Methoxybenzaldehyde, reactions 123-19-3, 4-Heptanone 123-38-6, Propionaldehyde, reactions 123-75-1, Pyrrolidine, reactions 134-20-3 141-75-3, Butyryl chloride 177-11-7, 1,4-Dioxa-8-azaspiro[4.5]decane 320-98-9, 5-Fluoro-2-nitrobenzoic acid 446-10-6, 4-Fluoro-2-nitrotoluene 500-22-1, Pyridine-3-carboxaldehyde 502-42-1, Cycloheptanone 503-29-7, Azetidine 583-60-8, 2-Methylcyclohexanone 583-68-6, 2-Bromo-4-methylaniline 585-71-7, (1-Bromoethyl)benzene 587-04-2, 3-Chlorobenzaldehyde 589-16-2, 4-Ethylaniline 610-14-0, 2-Nitrobenzoyl chloride 620-23-5 701-57-5, Methyl 4-nitrophenyl sulfide 765-43-5, Cyclopropylmethylketone 769-10-8, 2-Fluoro-6-nitrotoluene 872-85-5, 4-Pyridinecarboxaldehyde 873-38-1, 2-Bromo-4-chloroaniline 1003-04-9, Tetrahydrothiophen-3-one 1003-98-1, 2-Bromo-4-fluoroaniline 1008-91-9, 1-(4-Pyridyl)piperazine 1072-72-6, Tetrahydrothiopyran-4-one 1072-98-6, 2-Amino-5-chloropyridine 1120-72-5, 2-Methylcyclopentanone 1121-60-4, Pyridine-2-carboxaldehyde 1122-54-9, 4-Acetylpyridine 1126-09-6, Ethyl isonipecotate 1489-69-6, Cyclopropanecarboxaldehyde 1603-41-4, 2-Amino-5-methylpyridine 1710-98-1, 4-tert-Butylbenzoyl chloride 1776-53-0, 4-Aminocyclohexanecarboxylic acid 1793-07-3, 2-Carbomethoxyphenyl isocyanate 1882-69-5, 5-Methoxy-2-nitrobenzoic acid 2148-56-3, 2-Amino-6-chlorobenzoic acid 2366-70-3, 4,4,4-Trifluorobutan-2-one 2516-95-2, 5-Chloro-2-nitrobenzoic acid 3113-72-2, 5-Methyl-2-nitrobenzoic acid 3678-63-5, 4-Chloro-2-picoline 4315-09-7, 4-Nitroisophthalic acid 4363-93-3, Quinoline-4-carboxaldehyde 4771-47-5, 3-Chloro-2-nitrobenzoic acid 4786-20-3, 2-Butenenitrile 4897-84-1, Methyl 4-bromobutyrate 4920-80-3, 3-Methoxy-2-nitrobenzoic acid 5350-93-6 5372-81-6, 2-Aminoterephthalic acid dimethyl ester 5428-89-7, 2-Amino-5-chloropyrimidine 5437-38-7, 3-Methyl-2-nitrobenzoic acid 5469-69-2, 3-Amino-6-chloropyridazine 5470-22-4, 4-Chloropicolinic acid 5538-51-2, Acetylsalicylic acid chloride 6280-88-2, 4-Chloro-2-nitrobenzoic acid 7304-32-7, 2-Fluoro-5-nitrobenzoic acid 7379-35-3, 4-Chloropyridine hydrochloride 7486-35-3, Tributyl(vinyl)tin 10177-29-4, 4-Chloronicotinic acid 10200-59-6, Thiazole-2-carboxaldehyde 14002-51-8, 4-Biphenylcarbonyl chloride 17012-21-4, Methyl 1-benzylpyrrolidine-3-carboxylate 19235-89-3, 4-Chloro-2-cyanopyridine 19524-06-2 21717-96-4, 2-Amino-5-fluoropyridine 29943-42-8, Tetrahydro-4H-pyran-4-one 40499-83-0, 3-Hydroxypyrrolidine 55737-66-1, 4-Methoxycarbonyl-2-nitrobenzoic acid 57260-71-6, N-tert-Butoxycarbonylpiperazine 57946-63-1, 2-Bromo-4-trifluoromethylaniline 76143-33-4, 5-Methoxycarbonyl-2-nitrobenzoic acid 79099-07-3, 1-tert-Butoxycarbonyl-4-piperidone 84358-13-4, 1-tert-Butoxycarbonyl-isonipecotic acid 93913-86-1 103057-44-9, 1-tert-Butoxycarbonyl-3-hydroxypyrrolidine 109384-19-2, 1-tert-Butoxycarbonyl-4-hydroxypiperidine 118486-94-5, 2-(Tributylstannyl)furan 124252-41-1, 4-(Tributylstannyl)pyridine 141699-55-0, 1-tert-Butoxycarbonyl-3-hydroxyazetidine 173382-28-0

175278-17-8 183158-31-8 186550-13-0 218777-23-2
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280774-11-0 280774-12-1 280774-13-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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70684-84-3P 75541-82-1P 76842-15-4P 97776-06-2P
116721-57-4P 117145-55-8P 117145-66-1P 123855-51-6P,
1-tert-Butoxycarbonyl-4-hydroxymethylpiperidine
130234-74-1P 130309-46-5P 130658-67-2P 137076-22-3P,
1-tert-Butoxycarbonyl-piperidine-4-carboxaldehyde
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ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

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280774-08-5P 280774-09-6P 280774-15-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD.

REFERENCE(S):
(1) Beight Douglas Wade; WO 9900121 A 1999 CAPLUS
(2) Beight Douglas Wade; WO 9900128 A 1999 CAPLUS
(3) Berlex Lab; WO 9628427 A 1996 CAPLUS
(4) Katakura; EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY CHIMICA THERAPEUTICA 1995, V30(5), P387 CAPLUS
(5) Kunitada, S; CURRENT PHARMACEUTICAL DESIGN 1996, V2(5), P6
(6) Schering Ag; WO 9932477 A 1999 CAPLUS

=> d ibib abs 1

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:457059 CAPLUS
DOCUMENT NUMBER: 133:89437
TITLE: Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors
INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SOURCE: PCT Int. Appl., 403 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000039118	A1	20000706	WO 1999-US29946	19991215
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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ES 2226485	T3	20050316	ES 1999-964279	19991215
US 6635657	B1	20031021	US 2001-857751	20010608
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PRIORITY APPLN. INFO.:			US 1998-113556P P	19981223

WO 1999-US29946 W 19991215
US 2001-857751 A3 20010608

OTHER SOURCE(S): MARPAT 133:89437

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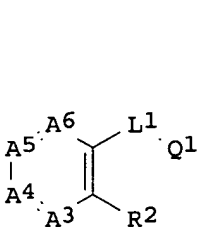

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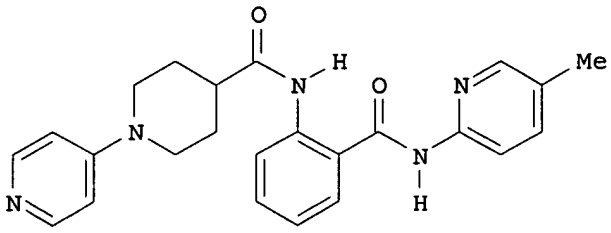

II

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REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE 'CAPLUS' ENTERED AT 14:11:14 ON 14 FEB 2006
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S L1

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L6 0 S L5
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FILE 'REGISTRY' ENTERED AT 14:12:25 ON 14 FEB 2006
L7 7 S L1 FULL

FILE 'CAPLUS' ENTERED AT 14:12:26 ON 14 FEB 2006
L8 5 S L7 FULL

=> d l8 ibib abs

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:457059 CAPLUS
DOCUMENT NUMBER: 133:89437
TITLE: Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors

INVENTOR(S): Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong

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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
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AT 272633	E	20040815	AT 1999-964279		19991215
ES 2226485	T3	20050316	ES 1999-964279		19991215
US 6635657	B1	20031021	US 2001-857751		20010608
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PRIORITY APPLN. INFO.:			US 1998-113556P	P	19981223
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OTHER SOURCE(S): MARPAT 133:89437

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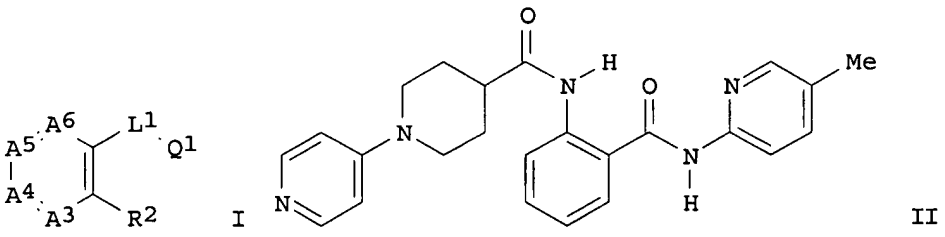

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=> 1
1 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d his

(FILE 'HOME' ENTERED AT 14:09:38 ON 14 FEB 2006)

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L1 STRUCTURE UPLOADED
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FILE 'REGISTRY' ENTERED AT 14:12:25 ON 14 FEB 2006
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YOU HAVE REQUESTED DATA FROM FILE 'REGISTRY' - CONTINUE? (Y)/N:y

'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats. The predefined substance formats
are: (RN = CAS Registry Number)

REG - RN
SAM - Index Name, MF, and structure - no RN
FIDE - All substance data, except sequence data
IDE - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD - Protein sequence data, includes RN
SQD3 - Same as SQD, but 3-letter amino acid codes are used
SQN - Protein sequence name information, includes RN

CALC - Table of calculated properties
EPROP - Table of experimental properties
PROP - EPROP and CALC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance. The substance formats

must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

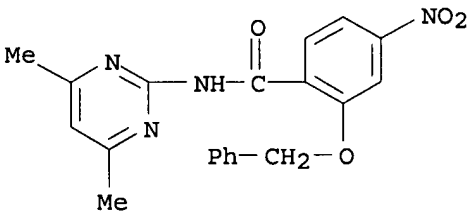
SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):ide

L7 ANSWER 1 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 856975-07-0 REGISTRY
ED Entered STN: 26 Jul 2005
CN Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H18 N4 O4
SR CAS EARLY REGISTRATIONS
LC STN Files: CA, CAPLUS

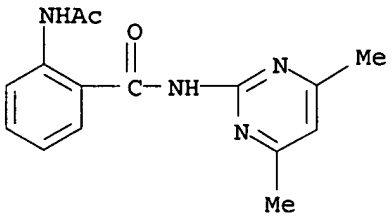


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 2 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 349622-99-7 REGISTRY
ED Entered STN: 01 Aug 2001
CN Benzamide, 2-(acetylamino)-N-(4,6-dimethyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H16 N4 O2
SR Chemical Library

Supplier: MicroChemistry Ltd.
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 ANSWER 3 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 280768-70-9 REGISTRY
ED Entered STN: 27 Jul 2000
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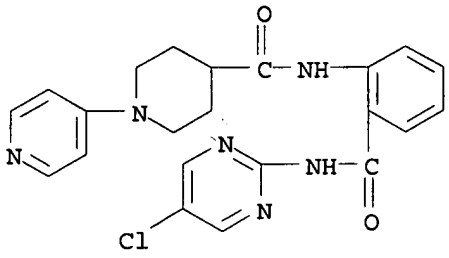

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 4 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 267891-53-2 REGISTRY
ED Entered STN: 02 Jun 2000
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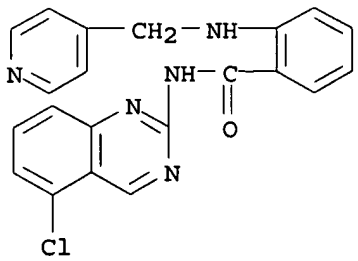
LC STN Files: CA, CAPLUS, TOXCENTER, USPAT2, USPATFULL



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ED Entered STN: 02 Jun 2000
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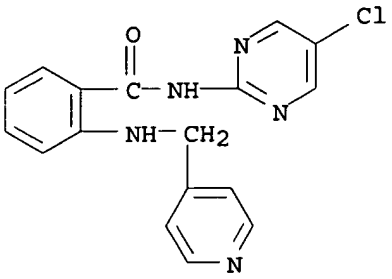

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 6 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 180206-29-5 REGISTRY
ED Entered STN: 29 Aug 1996
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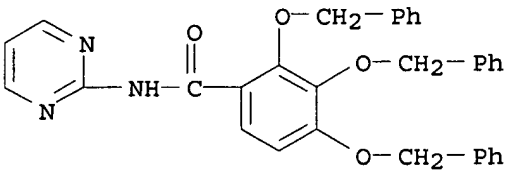

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 7 OF 7 REGISTRY COPYRIGHT 2006 ACS on STN
RN 69589-68-0 REGISTRY
ED Entered STN: 16 Nov 1984
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FS 3D CONCORD
MF C18 H14 N4 O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

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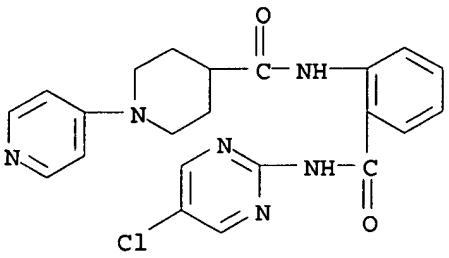
L6 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
IT **280768-70-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)
RN 280768-70-9 CAPLUS
CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phenyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)



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PATENT ASSIGNEE(S): Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
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FAMILY ACC. NUM. COUNT: 1
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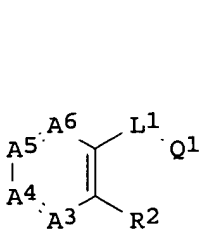

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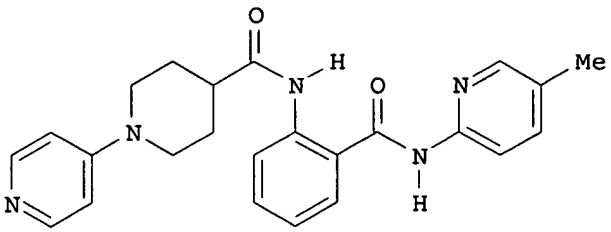


II

AB The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

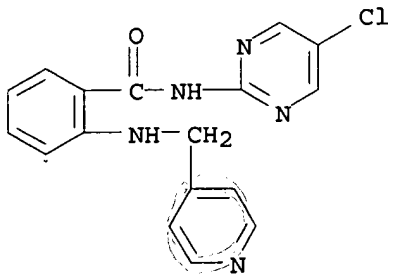
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

IT **267891-24-7P 267891-53-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

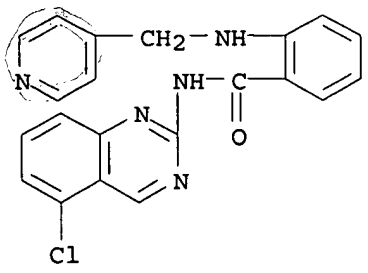
RN 267891-24-7 CAPLUS

CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 267891-53-2 CAPLUS

CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 2000:335387 CAPLUS
DOCUMENT NUMBER: 132:334364
TITLE: Preparation of anthranilic acid amides as vascular endothelial growth factor receptor inhibitors.
INVENTOR(S): Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz; Bold, Guido; Manley, Paul William; Furet, Pascal; Wood, Jeanette Marjorie; Mestan, Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard; Menrad, Andreas; Schirner, Michael
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany; Novartis Aktiengesellschaft
SOURCE: PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000027819	A2	20000518	WO 1999-EP8478	19991109
WO 2000027819	A3	20000817		
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19910396	A1	20000907	DE 1999-19910396	19990303
DE 19910396	C2	20011213		
CA 2350208	AA	20000518	CA 1999-2350208	19991109
BR 9915553	A	20010814	BR 1999-15553	19991109
EP 1129074	A2	20010905	EP 1999-953967	19991109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200101307	T2	20020521	TR 2001-200101307	19991109
JP 2002529452	T2	20020910	JP 2000-580999	19991109
EE 200100258	A	20021216	EE 2001-258	19991109
NZ 511413	A	20040130	NZ 1999-511413	19991109
AU 771180	B2	20040318	AU 2000-10454	19991109
NO 2001002245	A	20010710	NO 2001-2245	20010507
BG 105588	A	20020430	BG 2001-105588	20010611
HK 1041882	A1	20050318	HK 2002-103628	20020514

PRIORITY APPLN. INFO.:	GB 1998-24579	A	19981110
	DE 1999-19910396	A	19990303
	WO 1999-EP8478	W	19991109

OTHER SOURCE(S): MARPAT 132:334364
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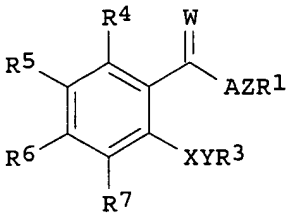
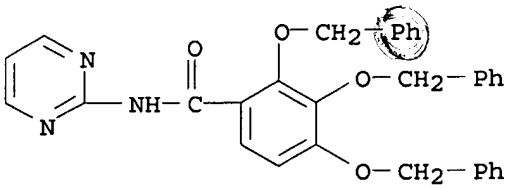


I

AB Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q, alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl, 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl; R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo, (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H,

• alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (preparation given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl)anthranilamide. The latter inhibited VEGFR I with IC50 = 0.05 μM.

L6 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
IT **180206-29-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)
RN 180206-29-5 CAPLUS
CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)



ACCESSION NUMBER: 1996:513596 CAPLUS
DOCUMENT NUMBER: 125:167581
TITLE: Preparation of hydroxybenzamide derivatives as prevention and treatment agents for bone diseases
INVENTOR(S): Nomoto, Takashi; Kawakami, Kumiko; Akagawa, Akiko; Matsuyama, Kenji; Torigoe, Koichiro
PATENT ASSIGNEE(S): Banyu Pharma Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08143525	A2	19960604	JP 1994-311235	19941121
PRIORITY APPLN. INFO.:			JP 1994-311235	19941121

OTHER SOURCE(S): MARPAT 125:167581
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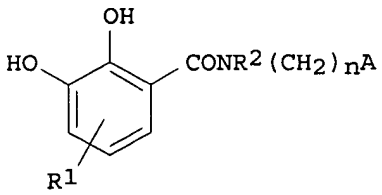
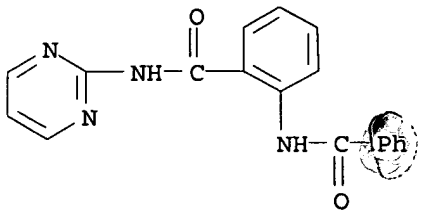


I

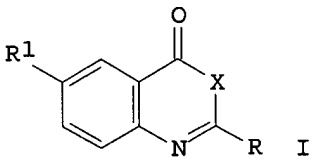
AB The title bone disease inhibitors contain a compound (I) [R1 = H, halo, OH, NO2, lower alkyl, lower alkoxy; R2 = H, lower alkyl; n = 0-3; A = aryl, heteroaryl; A and R2 may combine to complete piperidine or tetrahydroisoquinoline ring]. I is an efficient component for prevention and treatment of bone diseases caused by Vacuolar ATPase. Thus, 2,3,4-tribenzyloxybenzoic acid was reacted with aniline in the presence of 4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide, followed by hydrogenation to give I [R1 = OH; R2 = H; n = 0; A = Ph], 4 μM of which showed Vacuolar ATPase inhibiting activity of 97%.

L6 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
IT **69589-68-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 69589-68-0 CAPLUS
CN Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)

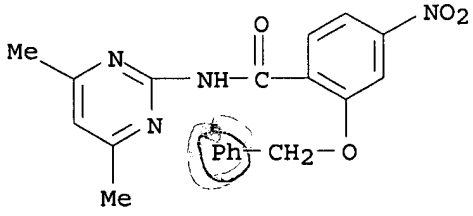


ACCESSION NUMBER: 1979:121516 CAPLUS
DOCUMENT NUMBER: 90:121516
TITLE: Condensation of acetanthranil and phenylanthranil with certain aminoheterocycles. Attempted preparation of some 2,3-disubstituted 4(3H)-quinazolinones
AUTHOR(S): El-Zanfally, S.
CORPORATE SOURCE: Fac. Pharm., Cairo Univ., Cairo, Egypt
SOURCE: Egyptian Journal of Pharmaceutical Sciences (1978), Volume Date 1976, 17(1), 29-34
CODEN: EJPSBZ; ISSN: 0301-5068
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 90:121516
GI



AB Treating 2-methyl-4H-3,1-benzoxazin-4-ones (I; X = O; R = Me; R1 = H, Br) with amines R2NH2 (R2 = 2-pyridyl, 4-antipyrinyl) yielded 35-81% the corresponding quinazolinones (I; X = NR2). The reactions were carried out by fusing the reactants at 150-60° for 3 h or by refluxing in pyridine-dioxane for 2 h. Similar reaction of I (X = O, R = Ph, R1 = H) with R2NH2 (R2 = 2-, 3-, or 4-pyridyl; 2-pyrimidinyl, or 4-antipyrinyl) gave o-R2NHCOC6H4NHCOPh.

L6 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
IT **856975-07-0**, Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl-
(preparation of)
RN 856975-07-0 CAPLUS
CN Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA INDEX NAME)



ACCESSION NUMBER: 1953:22216 CAPLUS
DOCUMENT NUMBER: 47:22216
ORIGINAL REFERENCE NO.: 47:3819d-i,3820a-i
TITLE: Tuberculostatic derivatives of p-aminobenzoic acid. III. Heterocyclic derivatives of 4-aminosalicylic acid
AUTHOR(S): Jensen, Kai Arne; Ingvorsen, Helmuth
CORPORATE SOURCE: Univ. Copenhagen
SOURCE: Acta Chemica Scandinavica (1952), 6, 161-5
CODEN: ACHSE7; ISSN: 0904-213X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and 4-aminosalicylic acid (II) were prepared, including 4-nitro-salicylomorpholide (III), m. 247-8°, and -piperidide (IV), m. 230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m. 170° and 4-aminobenzoic acid (VIII), m. 160°; 2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X), m. 178°, and -benzanilide (XI), m. 201°; 4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-nitrobenzamido)pyridine (XIII), m. 144°, -thiazole (XIV), m. 201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4-aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m. 214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et 4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at 120°, the excess XX removed at 100° in vacuo, the residue dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving 50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g. PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were refluxed until colorless, 0.2 N NaOH added until the color reappeared, the EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5 h., the excess SOCl2 was removed in vacuo, and the IX (9.2 g.) treated with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the solution filtered, part of the EtOH removed in vacuo, H2O added, the solution heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9 g. acid chloride. XVII to XIX were obtained by hydrogenation of the corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.

=>

L6 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:457059 CAPLUS
DN 133:89437
TI Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors
IN Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PA Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SO PCT Int. Appl., 403 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000039118	A1	20000706	WO 1999-US29946	19991215
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
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	CA 2361149	AA	20000706	CA 1999-2361149	19991215
	EP 1140903	A1	20011010	EP 1999-964279	19991215
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	JP 2002533454	T2	20021008	JP 2000-591029	19991215
	AT 272633	E	20040815	AT 1999-964279	19991215
	ES 2226485	T3	20050316	ES 1999-964279	19991215
	US 6635657	B1	20031021	US 2001-857751	20010608
	US 2004029874	A1	20040212	US 2003-629760	20030729
	US 6759414	B2	20040706		
	US 2005282862	A1	20051222	US 2003-629817	20030729
PRAI	US 1998-113556P	P	19981223		
	WO 1999-US29946	W	19991215		
	US 2001-857751	A3	20010608		

OS MARPAT 133:89437
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L6 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:457059 CAPLUS
DN 133:89437
TI Preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors
IN Beight, Douglas Wade; Craft, Trelia Joyce; Denny, Carl Penman; Franciskovich, Jeffry Bernard; Goodson, Theodore, Jr.; Hall, Steven Edward; Herron, David Kent; Joseph, Sajan Pariyadan; Klimkowski, Valentine Joseph; Masters, John Joseph; Mendel, David; Milot, Guy; Pineiro-Nunez, Marta Maria; Sawyer, Jason Scott; Shuman, Robert Theodore; Smith, Gerald Floyd; Tebbe, Anne Louise; Tinsley, Jennifer Marie; Weir, Leonard Crayton; Wikel, James Howard; Wiley, Michael Robert; Yee, Ying Kwong
PA Eli Lilly and Co., USA; Kyle, Jeffrey, Alan; et al.
SO PCT Int. Appl., 403 pp.
CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000039118	A1	20000706	WO 1999-US29946	19991215
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	CA 2361149	AA	20000706	CA 1999-2361149	19991215
	EP 1140903	A1	20011010	EP 1999-964279	19991215
	EP 1140903	B1	20040804		
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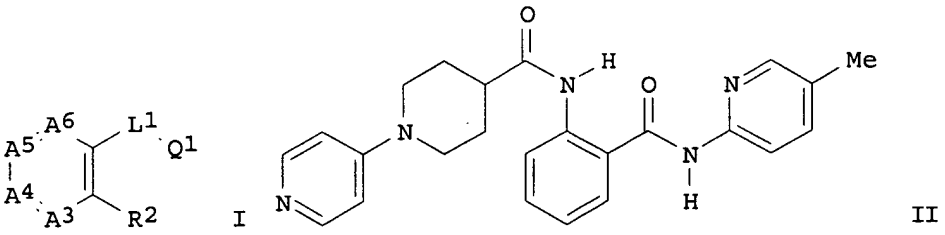
	JP 2002533454	T2	20021008	JP 2000-591029	19991215
	AT 272633	E	20040815	AT 1999-964279	19991215
	ES 2226485	T3	20050316	ES 1999-964279	19991215
	US 6635657	B1	20031021	US 2001-857751	20010608
	US 2004029874	A1	20040212	US 2003-629760	20030729
	US 6759414	B2	20040706		
	US 2005282862	A1	20051222	US 2003-629817	20030729
PRAI	US 1998-113556P	P	19981223		
	WO 1999-US29946	W	19991215		
	US 2001-857751	A3	20010608		

OS MARPAT 133:89437
GI

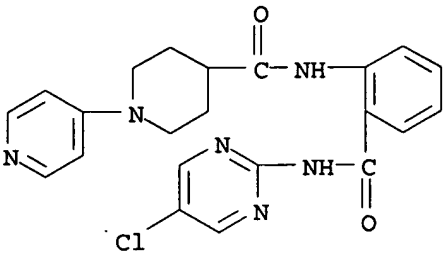


I II

AB The title compds. [I; A3-A6, together with the two carbons to which they are attached, complete a substituted benzene in which A3 = CR3, A4 = CR4, A5 = CR5, and A6 = CR6 (wherein R3 = H, Me, MeO, etc.; one of R4 and R5 = H, alkyl, halo, etc.; the other of R4 and R5 = H; R6 = H, Me, F, etc.); L1 = CONH; Q1 = 2-pyridinyl (un)substituted at the 5-position, 3-pyridinyl (un)substituted at the 6-position, 2-pyrimidinyl (un)substituted at the 5-position, etc.; R2 = L2Q2 (L2 = NHCO, NHCH2, OCH2, etc.; Q2 = (un)substituted piperidinyl, piperazinyl, Ph, etc.)] and their pharmaceutically acceptable salts, useful as inhibitors of factor Xa (no data), were prepared and formulated. E.g., a multi-step synthesis of II.HCl was given. In general, compds. I are effective at 0.01-1000 mg/kg/day.

IT **280768-70-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryl-substituted aromatic amides as factor Xa inhibitors)

RN 280768-70-9 CAPLUS
CN 4-Piperidinecarboxamide, N-[2-[[(5-chloro-2-pyrimidinyl)amino]carbonyl]phenyl]-1-(4-pyridinyl)- (9CI) (CA INDEX NAME)



RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 2000:335387 CAPLUS
DN 132:334364
TI Preparation of anthranilic acid amides as vascular endothelial growth factor receptor inhibitors.
IN Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz; Bold, Guido; Manley, Paul William; Furet, Pascal; Wood, Jeanette Marjorie; Mestan, Jurgen; Bruggen, Jose; Ferrari, Stefano; Kruger, Martin; Ottow, Eckhard; Menrad, Andreas; Schirner, Michael
PA Schering Aktiengesellschaft, Germany; Novartis Aktiengesellschaft
SO PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000027819	A2	20000518	WO 1999-EP8478	19991109
	WO 2000027819	A3	20000817		
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	DE 19910396	A1	20000907	DE 1999-19910396	19990303
	DE 19910396	C2	20011213		
	CA 2350208	AA	20000518	CA 1999-2350208	19991109
	BR 9915553	A	20010814	BR 1999-15553	19991109
	EP 1129074	A2	20010905	EP 1999-953967	19991109
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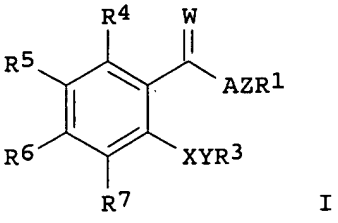
	TR 200101307	T2	20020521	TR 2001-200101307	19991109
	JP 2002529452	T2	20020910	JP 2000-580999	19991109
	EE 200100258	A	20021216	EE 2001-258	19991109
	NZ 511413	A	20040130	NZ 1999-511413	19991109
	AU 771180	B2	20040318	AU 2000-10454	19991109
	NO 2001002245	A	20010710	NO 2001-2245	20010507
	BG 105588	A	20020430	BG 2001-105588	20010611
	HK 1041882	A1	20050318	HK 2002-103628	20020514
PRAI	GB 1998-24579	A	19981110		
	DE 1999-19910396	A	19990303		
	WO 1999-EP8478	W	19991109		

OS MARPAT 132:334364
GI



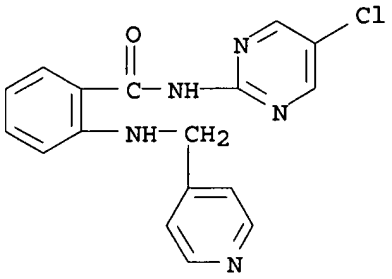
I

AB Title compds. [I; A = NR2; W = O, S, H2, NR8; Z = NR10, N, NR10(CH2)q, alkyl, etc.; q = 1-6; AZR1 = tetrahydroisoquinolinyl, indazolyl, 5-chloroindolyl, etc.; R1 = (substituted) aryl, heteroaryl; R2 = H, alkyl; R3 = (substituted) mono- or bicyclic aryl, heteroaryl; R4-R7 = H, halo, (substituted) alkoxy, alkyl, carboxyalkyl; R5R6 = dioxetanyl; R8, R10 = H, alkyl]. Thus, Me N-(4-pyridylmethyl)anthranilate (preparation given) was stirred with Ph(CH2)3NH2 and Me3Al were stirred in PhMe to give N-(3-phenylprop-1-yl)-N2-(4-pyridylmethyl)anthranilamide. The latter inhibited VEGFR I with IC50 = 0.05 μM.

IT **267891-24-7P 267891-53-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of anthranilic acid amides as VEGF receptor inhibitors)

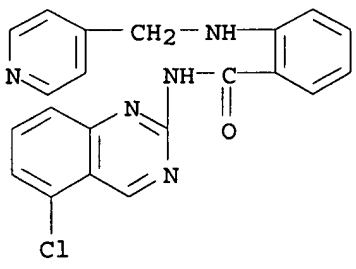
RN 267891-24-7 CAPLUS

CN Benzamide, N-(5-chloro-2-pyrimidinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)



RN 267891-53-2 CAPLUS

CN Benzamide, N-(5-chloro-2-quinazolinyl)-2-[(4-pyridinylmethyl)amino]- (9CI) (CA INDEX NAME)



L6 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:513596 CAPLUS

DN 125:167581

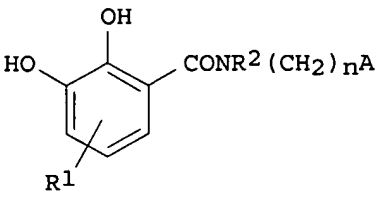
TI Preparation of hydroxybenzamide derivatives as prevention and treatment agents for bone diseases

IN Nomoto, Takashi; Kawakami, Kumiko; Akagawa, Akiko; Matsuyama, Kenji; Torigoe, Koichiro

PA Banyu Pharma Co Ltd, Japan
SO Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 08143525	A2	19960604	JP 1994-311235	19941121
PRAI	JP 1994-311235		19941121		

OS MARPAT 125:167581
GI

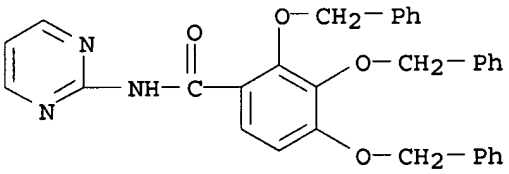


I

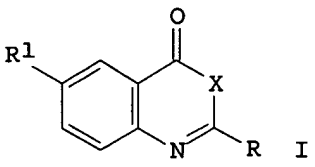
AB The title bone disease inhibitors contain a compound (I) [R1 = H, halo, OH, NO2, lower alkyl, lower alkoxy; R2 = H, lower alkyl; n = 0-3; A = aryl, heteroaryl; A and R2 may combine to complete piperidine or tetrahydroisoquinoline ring]. I is an efficient component for prevention and treatment of bone diseases caused by Vacuolar ATPase. Thus, 2,3,4-tribenzyloxybenzoic acid was reacted with aniline in the presence of 4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide, followed by hydrogenation to give I [R1 = OH; R2 = H; n = 0; A = Ph], 4 μM of which showed Vacuolar ATPase inhibiting activity of 97%.

IT **180206-29-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of hydroxybenzamide derivs. as Vacuolar ATPase inhibitors)

RN 180206-29-5 CAPLUS
CN Benzamide, 2,3,4-tris(phenylmethoxy)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)



L6 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
AN 1979:121516 CAPLUS
DN 90:121516
TI Condensation of acetanthranil and phenylanthranil with certain aminoheterocycles. Attempted preparation of some 2,3-disubstituted 4(3H)-quinazolinones
AU El-Zanfally, S.
CS Fac. Pharm., Cairo Univ., Cairo, Egypt
SO Egyptian Journal of Pharmaceutical Sciences (1978), Volume Date 1976, 17(1), 29-34
CODEN: EJPSBZ; ISSN: 0301-5068
DT Journal
LA English
OS CASREACT 90:121516
GI

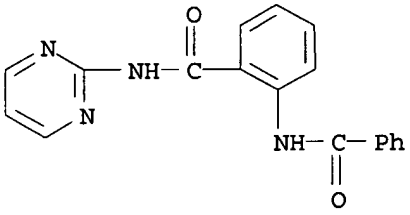


AB Treating 2-methyl-4H-3,1-benzoxazin-4-ones (I; X = O; R = Me; R1 = H, Br) with amines R2NH2 (R2 = 2-pyridyl, 4-antipyrinyl) yielded 35-81% the corresponding quinazolinones (I; X = NR2). The reactions were carried out by fusing the reactants at 150-60° for 3 h or by refluxing in pyridine-dioxane for 2 h. Similar reaction of I (X = O, R = Ph, R1 = H) with R2NH2 (R2 = 2-, 3-, or 4-pyridyl; 2-pyrimidinyl, or 4-antipyrinyl) gave o-R2NHCOC6H4NHCOPh.

IT **69589-68-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 69589-68-0 CAPLUS

CN Benzamide, 2-(benzoylamino)-N-2-pyrimidinyl- (9CI) (CA INDEX NAME)



L6 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1953:22216 CAPLUS

DN 47:22216

OREF 47:3819d-i,3820a-i

TI Tuberculostatic derivatives of p-aminobenzoic acid. III. Heterocyclic derivatives of 4-aminosalicylic acid

AU Jensen, Kai Arne; Ingvorsen, Helmuth

CS Univ. Copenhagen

SO Acta Chemica Scandinavica (1952), 6, 161-5
CODEN: ACHSE7; ISSN: 0904-213X

DT Journal

LA English

AB cf. C.A. 43, 7454i. A number of heterocyclic derivs. of 4-nitro- (I) and 4-aminosalicylic acid (II) were prepared, including 4-nitro-salicylomorpholide (III), m. 247-8°, and -piperidide (IV), m. 230-2°; 4-aminosalicylomorpholide (V), m. 161-2°, and -piperidide (VI), m. 134-5°; 2-benzyloxy-4-nitro-(VII), m. 170° and 4-aminobenzoic acid (VIII), m. 160°; 2-benzyloxy-4-nitrobenzoyl chloride (IX), m. 122°, -benzamide (X), m. 178°, and -benzanilide (XI), m. 201°; 4-amino-salicylanilide (XII), m. 143°; 2-(2-benzyloxy-4'-nitrobenzamido)pyridine (XIII), m. 144°, -thiazole (XIV), m. 201° -5-methyl-1,3,4-thiadiazole (XV), m. 196°, and -4,6-dimethylpyrimidine (XVI), m. 206°; and 2-(2-benzyloxy-4-aminobenzamido)pyridine (XVII), m. 183°, -thiazole (XVIII), m. 214-15°, and -5-methyl-1,3,4-thiazole (XIX), m. 110-11°. Et 4-nitrosalicylate (3 g.) and 3 g. morpholine (XX) were heated 5 h. at 120°, the excess XX removed at 100° in vacuo, the residue dissolved in hot H2O, acidified with HOAc, and the solution cooled, giving

50% III. IV was similarly prepared III (0.5 g.) hydrogenated with 0.01 g. PtO2 in 25 cc. EtOH, all of the EtOH removed in vacuo, and fractional crystallization of the residue from petr. ether gave 0.2 g.V. VI was similarly prepared I (50 g.), 35 g. PhCH2Cl, and 50 cc. 20% NaOH in 100 cc. EtOH were refluxed until colorless, 0.2 N NaOH added until the color reappeared, the EtOH distilled, H2O added, and dilute HCl added to complete the precipitation of VII (40 g.). VII hydrogenated over PtO2 with the amount of H calculated for reduction of the NO2 gave VIII. VII (10 g.) and 10 cc. SOCl2 were refluxed 1-1.5 h., the excess SOCl2 was removed in vacuo, and the IX (9.2 g.) treated with C and recrystd. from C6H6; 2 g. IX and 10 cc. cold, concentrated aqueous NH3 in 30 cc. H2O neutralized with HOAc gave 1.3 g. X (from 90% EtOH). IX (2.9 g.), 1 g. PhNH2, and 5 cc. pyridine were cooled and the mixture poured into 300 cc. H2O, giving 2.2 g. XI (from HOAc). XI hydrogenated in EtOH, the solution filtered, part of the EtOH removed in vacuo, H2O added, the solution heated, charcoal added, and the hot solution filtered gave XII. XIII to XVI were prepared like VII, in 2.2, 2.7, 1.7, and 1.7 g. yields, resp., from 2.9 g. acid chloride. XVII to XIX were obtained by hydrogenation of the corresponding nitro compds. over PtO2 in EtOH. Hydrogenation of the nitro compds. at 100° and 150 atmospheric gave the corresponding azoxy compds.

IT **856975-07-0**, Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl-
(preparation of)

RN 856975-07-0 CAPLUS

CN Pyrimidine, 2-[2-(benzyloxy)-4-nitrobenzamido]-4,6-dimethyl- (5CI) (CA INDEX NAME)